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RESEARCH REPORT No. CX-29

A Variational Calculation of the Scattering Cross Section for Nearly Zero-Energy Electrons by Hydrogen Atoms

HOWARD GREENBERG and SIDNEY BOROWITZ

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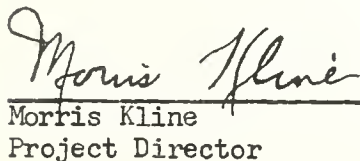
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A VARIATIONAL CALCULATION OF THE SCATTERING CROSS SECTION
FOR NEARLY ZERO ENERGY ELECTRONS BY HYDROGEN ATOMS

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Abstract

The cross section for the scattering of electrons by hydrogen atoms at zero energy has been calculated using a variational principle of the Hulthen-Kohn type. For singlet scattering we have used a three parameter trial function which reduces to an H^- wave function at small electron separations and which has the correct asymptotic form. To calculate triplet scattering we use an antisymmetrized version of the same trial function. The effective range for singlet scattering is determined from the scattering length already calculated and the known value of the electron attachment energy for H^- . For triplet scattering we use an energy-dependent trial function to determine the effective range. Using the calculated values of the above parameters we find the cross section as a function of energy for the range 0 - 0.02 volts. The values of the cross section are then used to calculate the resistivity of silicon alloys due to neutral impurity scattering.

Table of Contents

	<u>Page</u>
1. Introduction	1
2. The variational principle	5
3. Dependence of the scattering on the energy of the incident electron	16
A. Effective range theory	16
B. Independent calculation of r_0	21
4. Sensitivity of the method	24
5. Neutral impurity scattering in semiconductors	28
Appendix I. Calculation of variational parameters using $\Psi_t = \Phi + \chi$	31
Appendix II. Calculation of variational parameters using $\Psi_t = (1 + cr_{12}) \Phi + \chi$	35
Appendix III. Calculations required for r_{os} and r_{ot} with energy-dependent trial functions	39
Graphs	44
References	49

Table of Contents

	<u>Page</u>
1. Introduction	1
2. The variational principle	5
3. Dependence of the scattering on the energy of the incident electron	16
A. Effective range theory	16
B. Independent calculation of r_0	21
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5. Neutral impurity scattering in semiconductors	28
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Appendix II. Calculation of variational parameters using $\Psi_t = (1 + cr_{12}) \Phi + \chi$	35
Appendix III. Calculations required for r_{os} and r_{ot} with energy-dependent trial functions	39
Graphs	44
References	49

1. Introduction

The scattering of low-energy electrons by atomic systems is of some interest as one of the fundamental processes which occur in ionospheric and astrophysical phenomena. More detailed knowledge of the scattering process would also be of great aid in understanding certain aspects of gas discharges.

The simplest case of this sort is the scattering of electrons by hydrogen atoms. Measurements of the cross section for this system have been made by Bederson^[1] in the energy range above 2 volts. However, experiments for the energy range from zero electron energy to thermal energy, a range of practical interest, are extremely difficult to carry out. At present there exists no data for this energy range.

In order to gain some knowledge of the low-energy scattering it is necessary to carry out a theoretical calculation. The problem of the scattering of electrons by hydrogen atoms is a three-body problem and thus not amenable to exact solution. One is therefore compelled to seek approximate methods of solution.

The first attempts to solve the problem consisted in replacing the three-body problem by the scattering of an electron by a center force. One thus considered the scattering of electrons by a Hartree field or by a Fermi-Thomas statistical potential. These approximations suffered from some serious deficiencies. For one thing they did not take account of the polarization of the atom by the field of the incident electron, nor did they adequately provide for the consideration of exchange effects which are extremely important for low-energy scattering.

McDougall^[17] and Chandrasekhar and Breen^[9] have treated low-energy electron-hydrogen atom scattering in the one-body approximation using the method of partial waves to calculate the cross section.

The need for more accurate approximation methods has led to a study of the applicability of variational techniques to collision problems.

Schwinger^[22] has developed very powerful techniques which are based on converting the Schrödinger differential equation into an integral equation involving a Green's function appropriate to the particular collision problem under consideration. These methods give stationary expressions for the scattered amplitude and the phase shifts. These techniques have been extended by Borowitz and Friedman^[4] to handle three-body collisions.

Other variational techniques based on the differential equation have been developed by Hulthén^[13]. Kohn^[15] has developed variational techniques for many-body collision problems. Kato^[14] has developed a variational procedure which gives upper and lower bounds on the phase shifts for one-body collisions. However, methods for obtaining bounds for the phase shifts for three-body collisions are still lacking.

The variational methods have been applied to the calculation of the electron-hydrogen atom scattering cross section by numerous authors. Massey and Moiseiwitsch^{[18], [19]} have used the methods of Hulthén and Kohn to calculate the elastic scattering cross section of electrons by hydrogen atoms. Huang^[12] has developed his own technique and applied it to electron-hydrogen atom collisions, taking polarization into account but neglecting exchange effects. Massey and Moiseiwitsch have shown how to modify Huang's method so as to consider exchange effects. Boyet and Borowitz^[6] have applied the Schwinger method^[22] to

calculate the direct scattered amplitude for elastic collisions of electrons with hydrogen atoms. Moiseiwitsch^[20] has extended Hulthén's procedure to inelastic processes and has determined the phase shift for the 1S-2S excitation of hydrogen atoms by electrons.

None of the above calculations are well suited for the range near zero incident electron energy. The Hulthén-Kohn variational calculations appear to offer a better approach to problems in this energy range than other techniques. Born approximation procedures, for example, are good only for high-energy scattering, and the Schwinger variational method^[5] leads to integrals which cannot be easily evaluated (cf. [5]).

In a similar nuclear scattering problem, namely that of low-energy neutron-proton scattering, Schwinger^[22] has shown that the bound state of the deuteron lying near the continuum gives the dominant contribution to the cross section. The same situation should hold for the case of low-energy electron-hydrogen atom scattering, since there is a bound state of the H^- ion lying about three quarters of a volt below the continuum^{[7],[8]}. By using a variational method with a trial function suitable for the H^- ion we probably include all of the polarization effects when the low-energy electron is close to the hydrogen atom. The bound state of H^- is a singlet state, so that we have no similar guide for choosing a trial function for the triplet scattering. However, this choice is not crucial, as we shall show that the singlet scattering is the dominant feature in the process.

It is the purpose of this paper to make an accurate calculation of the cross section at zero incident electron energy. We shall then use the effective range theory^{[2],[3]} to find the cross section at small but finite electron energies.

In Section 2 we define the phase shifts for three-body scattering by using the S-matrix formalism. We show there that the phase shifts are defined only if the space part of the wave function is symmetric or anti-symmetric in the coordinates of the electrons. We then extend the Kohn-Hulthén variational principle to three-body collisions. Using this method we calculate the singlet and triplet scattering lengths. From these results we calculate the total cross section for zero-energy incident electrons.

In Section 3 we extend the effective range theory to three-body collisions. Using the fact that a bound state of H^- exists we calculate the effective range for the singlet scattering. We next introduce an energy-dependent trial function and use it to find the effective range for triplet scattering.

With these results we calculate the total cross section for incident electron energies between zero and thermal energies.

In Section 4 we compare our results with the extrapolated results of Massey and Moiseiwitsch^[19] for the same energy range. We then discuss the sensitivity of the cross section to the parameters which appear in the effective range theory. Finally we obtain an estimate of the accuracy of our calculation.

Erginsoy^[11] has used the scattering of electrons by hydrogen atoms as a model to explain the effect of neutral impurities on the resistivity of semiconductors at low temperatures. In Section 5 we use our improved values of the cross section to calculate the resistivity at low temperatures and compare these with the values obtained by Erginsoy using the cross sections of Massey and Moiseiwitsch^[18].

2. The variational principle

We begin by considering the three-body wave equation for S-wave scattering with the origin of coordinates at one of the particles whose mass we assume infinite. This equation is

$$(1) \quad L \Psi(\vec{r}_1, \vec{r}_2) = 0$$

where L is the operator

$$(2) \quad L = \frac{\hbar^2}{2m_1} \nabla_1^2 + \frac{\hbar^2}{2m_2} \nabla_2^2 - \left[V(\vec{r}_1, \vec{r}_2) - E \right] ;$$

here \vec{r}_1 and \vec{r}_2 are the distances of particles 1 and 2 from the origin, m_1 and m_2 are the masses of the electrons, \hbar is Planck's constant divided by 2π , V is the potential energy of the system, $\frac{\hbar^2}{2m} \nabla^2$ is the kinetic energy operator and E is the total energy of the system. For the case of scattering of electrons by hydrogen atoms (1) becomes, after some rearrangement of terms

$$(3) \quad \left[\nabla_1^2 + \nabla_2^2 + 2 \left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} - \frac{1}{2} + \frac{k^2}{2} \right) \right] \Psi(\vec{r}_1, \vec{r}_2) = 0 ,$$

where k is the wave number of the incident electron. We have set $m_1 = m_2 = m =$ the mass of the electron. We have chosen units such that $e = m = \hbar = 1$, where e is the charge of the electron. In these units the radius of the first Bohr orbit is equal to unity and the binding energy of an electron in the ground state of a hydrogen atom is $E_H = -\frac{1}{2}$.

The meaning of the other quantities may be seen from Figure 1.

We shall now rederive the Kato principle for the case of three-body scattering and apply it to low-energy electron-hydrogen atom scattering.

Before proceeding, however, it will be necessary to generalize the phase shift analysis to the problem of three-body scattering.

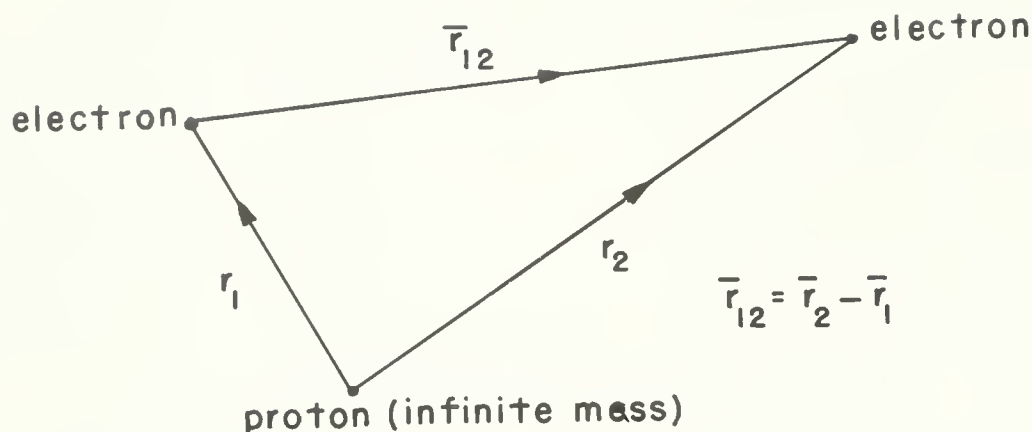


Figure 1

For two-body scattering with central forces the diagonal elements of the S-matrix are related to the phase shift by

$$(4) \quad S_{jj} = e^{2i\delta_j} \quad .$$

For this case the spherical harmonics are a representation in which the S-matrix is diagonal.

For the case of two-body scattering with tensor forces the S-matrix is no longer diagonal in this representation. In order to define the phase shift we must therefore diagonalize the S-matrix. Schwinger has shown for the problem of neutron-proton scattering with tensor forces that the eigenvalues of the S-matrix are related to the phase shifts by the relation given in (4). We can define a phase shift generally in terms of the diagonal elements of the S-matrix by equation (4). In the case of the scattering of electrons by hydrogen atoms, the spherical harmonics do not form a basis for diagonalizing the S-matrix because of exchange scattering.

In order to diagonalize the S-matrix we follow the method due to Kohn who has shown that the asymptotic form of the wave equation for an electron colliding with an atomic system can be written as

$$(5) \quad \Psi^{(\mu)} = \sum_i \phi_i P_i N_i \left[a_i^{(\mu)} \frac{e^{-ikr_i}}{r_i} - \beta_i^{(\mu)} \frac{e^{ikr_i}}{r_i} \right]$$

where P_i is the angular part of the wave function, N_i is a normalization constant, and ϕ_i is the normalized ground-state wave function for the atom. The index i runs over 1 or 2 and distinguishes the coordinates of each electron. The superscript $\mu = 1, 2$, refers to the two different modes of collisions which can occur, depending on whether electron 1 or 2 is incident.

The S-matrix is now defined by the relation

$$(6) \quad \beta_i^\mu = \sum_j S_{ij} a_j^\mu .$$

For the case of the scattering of electrons by hydrogen atoms we may choose two Ψ , whose asymptotic forms are

$$(7) \quad \Psi^{(1)} = N_1 P_1 \left[\left(\frac{e^{-ikr_1}}{r_1} - (1+2ikf) \frac{e^{ikr_1}}{r_1} \right) \phi_o(r_2) - 2ikg \frac{e^{ikr_2}}{r_2} \phi_o(r_1) \right]$$

$$(8) \quad \Psi^{(2)} = N_2 P_2 \left[\left(\frac{e^{ikr_2}}{r_2} - (1+2ikf) \frac{e^{ikr_2}}{r_2} \right) \phi_o(r_1) - 2ikg \frac{e^{ikr_1}}{r_1} \phi_o(r_2) \right] ,$$

where $\Psi^{(1)}$ is the wave function for particle 1 incident with particle 2 bound and $\Psi^{(2)}$ is that for particle 2 incident and particle 1 bound. $\phi_o(r_1)$ and $\phi_o(r_2)$ are the normalized ground state hydrogen atom wave functions, and f and g are the direct and exchange scattered amplitudes.

The elements of the S-matrix are clearly

$$(10) \quad \begin{cases} S_{11} = S_{22} = 1 + 2ikf \\ S_{12} = S_{21} = 2ikg \end{cases} .$$

We must now find the linear combinations of $\Psi^{(1)}$ and $\Psi^{(2)}$ which make the S-matrix diagonal.

The unitary matrix that diagonalizes the S-matrix is

$$(11) \quad U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} .$$

The particular linear combinations which diagonalize the S-matrix are then found from the relation

$$(12) \quad U \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} \Psi^{(1)} \\ \Psi^{(2)} \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} \Psi^{(1)} + \Psi^{(2)} \\ \Psi^{(1)} - \Psi^{(2)} \end{pmatrix} .$$

Thus the space wave functions which describe the scattering must be either symmetric or antisymmetric in the coordinates r_1 and r_2 .

The eigenvalues of the S-matrix are now easily found by using the relation

$$(13) \quad S_{jj} = U S U^{-1}$$

and are given by relations

$$(14) \quad S_{11} = e^{2i\delta_1} = 1 + 2ik(f + g),$$

$$(15) \quad S_{22} = e^{2i\delta_2} = 1 + 2ik(f - g) .$$

From the above discussion we see that the scattering is described by two phase shifts δ_1 and δ_2 corresponding to the symmetric and antisymmetric wave functions respectively.

We now proceed to the generalization of the Kato variational principle. Consider the integral

$$(16) \quad I = \int (uLv - vLu) d\tau_1 d\tau_2 ,$$

where $L = E - H$. H is the Hamiltonian for the system and E is the total energy.

Equation (16) can now be written as

$$(17) \quad \begin{aligned} I &= \int \left[u(\nabla_1^2 + \nabla_2^2)v - v(\nabla_1^2 + \nabla_2^2)u \right] d\tau_1 d\tau_2 \\ &= \int \left[u\nabla_1^2 v - v\nabla_1^2 u \right] d\tau_1 d\tau_2 + \int \left[u\nabla_2^2 v - v\nabla_2^2 u \right] d\tau_1 d\tau_2 . \end{aligned}$$

The application of Green's theorem gives

$$(18) \quad I = \int \left[u\nabla_1 v - v\nabla_1 u \right] dS_1 d\tau_2 + \int \left[u\nabla_2 v - v\nabla_2 u \right] dS_2 d\tau_1 ,$$

where ∇_1 and ∇_2 are the usual gradient operators, dS_1 and dS_2 are the surface elements of spheres in r_1 - and r_2 -space at infinity.

Let us now choose $u = \Psi$ to be a solution of (1), that is, $L\Psi = 0$, and we choose $v = \Psi_t$. Ψ_t is chosen so as to have the same asymptotic form as Ψ except that it may differ in phase.

We take the asymptotic forms for Ψ and Ψ_t as

$$(19) \quad \Psi \rightarrow \frac{1}{\gamma 8\pi} \frac{1}{r_1} \left[\cos(kr_1 + \theta) + \lambda_\theta \sin(kr_1 + \theta) \right] \phi_0(r_2) \quad r_1 \rightleftharpoons r_2 ,$$

$$(20) \quad \Psi_t \rightarrow \frac{1}{\gamma 8\pi} \frac{1}{r_1} \left[\cos(kr_1 + \theta) + \lambda_{\theta_t} \sin(kr_1 + \theta) \right] \phi_0(r_2) \quad r_1 \rightleftharpoons r_2 ,$$

where

$$(21) \quad \begin{cases} \lambda_{\theta} = \cot(\delta - \theta) \\ \lambda_{\theta_t} = (\cot \delta_t - \theta) \end{cases} ;$$

here δ is the phase shift. From the previous discussion we see that two phase shifts are defined: one for the symmetric wave function and one for the anti-symmetric wave function, so that we shall have a variational principle for each phase shift.

If we now insert equations (19) and (20) into (18), and use (16), we obtain the result

$$(22) \quad k(\lambda_{\theta_t} - \lambda_{\theta}) = \int \Psi L \Psi_t d\tau_1 d\tau_2 .$$

If we now let $w = \Psi - \Psi_t$, equation (22) becomes

$$(23) \quad k\lambda_{\theta} = k\lambda_{\theta_t} - \int \Psi_t L \Psi_t d\tau_1 d\tau_2 + \int w L w d\tau_1 d\tau_2$$

or

$$(24) \quad k \cot(\delta - \theta) = k \cot(\delta_t - \theta) - \int \Psi_t L \Psi_t d\tau_1 d\tau_2 + \int w L w d\tau_1 d\tau_2 .$$

The last term on the right is of second order in the error $\Psi - \Psi_t$, so that (24) is a variational principle for $k \cot(\delta - \theta)$. If we now set $\theta = 0$, then (24) reduces to the Kohn-Hulthén principle

$$(25) \quad k \cot \delta = k \cot \delta_t - \int \Psi_t L \Psi_t d\tau_1 d\tau_2$$

which is the form of the variational principle we shall use in our calculations.

We shall now apply (25) to the calculation of $k \cot \delta$ for the scattering of zero-energy electrons by hydrogen atoms. Equation (3) then reduces to

$$(26) \quad \left[\nabla_1^2 + \nabla_2^2 + 2\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} - \frac{1}{2}\right) \right] \Psi(\vec{r}_1, \vec{r}_2) = 0 .$$

The trial functions which we choose for use in the variational principle must be chosen so as to have the correct asymptotic form as given by equation (20). Furthermore, in order to define the phase shifts the trial functions must be symmetric or antisymmetric in their space coordinates r_1 and r_2 .

We point out here that the trial functions used by Massey and Moiseiwitsch^[19] in their one-body and polarization approximations and the trial function used by Huang do not have the proper symmetry, so that the phase shifts can not be defined. The use of these trial functions for the calculation of the phase shifts therefore leads to meaningless results.

Since we are dealing with electrons, the total wave function (space and spin) must be antisymmetric in the space and spin coordinates of both electrons in order to satisfy the Pauli principle. For the case of the symmetric space wave function the electron spins must be aligned antiparallel (singlet scattering), while for the antisymmetric space wave function the electron spins will be aligned parallel (triplet scattering).

From the previous discussion we can therefore define two phase shifts, one for the singlet and one for the triplet scattering.

It is well known that a bound state of H^- exists. In the H^- ion the electrons have their spins aligned antiparallel (singlet state). Chandrasekhar^[8] has used the Ritz method with a trial function of the form

$$e^{-\alpha r_1} e^{-\beta r_2} + e^{-\beta r_1} e^{-\alpha r_2}$$

to calculate the binding energy of the second electron in the ion; his result is 0.7019 volts.

In choosing a trial function for our phase shift calculation for the singlet scattering, we should like it to reduce to the trial function of

Chandrasekhar^[8] when both the electrons are close to the nucleus. When the incident electron is far from the hydrogen atom we should like the trial function to have the correct asymptotic form. For the case under consideration this will be the product of a normalized ground state hydrogen atom wave function with the sum of an incident plane wave and a scattered wave. With these considerations in mind we choose the following trial function:

$$(27) \quad \Psi_t = A \left[e^{-\alpha r_1} e^{-\beta r_2} + e^{-\alpha r_2} e^{-\beta r_1} \right] + \frac{1}{\sqrt{8} \pi} \left[B(1 - e^{-\gamma r_2}) + \frac{(1 - e^{-\gamma r_2})^2}{r_2} \right] e^{-r_1} + r_1 \rightleftharpoons r_2 ,$$

where the factor containing A is called Φ and the remainder is χ . A, B and γ are the parameters to be varied and $1/\sqrt{8} \pi$ is a normalization constant. In the present calculation we shall assume α and β are constant and use the values obtained by Chandrasekhar, namely, $\alpha = 1.03925$ and $\beta = 0.28309$.

We note that in order to get the most accurate results, α and β should also be varied. However, if this is done the numerical calculations involved become too burdensome.

The symmetric form of (27) will describe the singlet scattering. For the triplet scattering we shall use the antisymmetric form of (27).

If we substitute equations (26) and (27) into (25), it takes the form

$$(28) \quad X_o = \lim_{k \rightarrow 0} (k \cot \delta) = - \left[a_o A^2 + b_o B^2 + c_o AB + d_o + e_o A + (f_o - 1)B \right]$$

where $B = k \cot \delta_t$.

We must now make (28) an extremum with respect to A, B and γ .

The conditions $\partial X_o / \partial A = \partial X_o / \partial B = 0$ yield the relations

$$(29) \quad 2a_o A + c_o B + e_o = 0$$

$$(30) \quad c_o A + 2b_o B + (f_o - 1) = 0 ,$$

which give for A and B

$$(31) \quad A = \frac{c_o(f_o - 1) - 2b_o e_o}{4a_o b_o - c_o^2}$$

$$(32) \quad B = \frac{c_o e_o - 2a_o(f_o - 1)}{4a_o b_o - c_o^2} .$$

The quantities a_o , b_o , etc. are functions of γ , which are obtained by evaluating the integrals which occur when we substitute equations (26) and (27) into equation (25). This involves the evaluation of a great many integrals, most of which are elementary in nature. These calculations, straightforward but quite lengthy, are given in Appendix I. Once the quantities a_o , b_o ,... are obtained as functions of γ we can calculate X_o as a function of γ numerically, subject to the conditions (31) and (32), and look for the value of γ which makes (28) an extremum.

The numerical calculations involved were carried out with the aid of the Burroughs E101 digital computer. The results are summarized in Table I:

	<u>Table I</u>			
	X_o	γ	A	B
Singlet	-0.1226	0.12	0.0414	-0.1282
Triplet	-0.4251	0.46	0.00557	-0.4256

The trial wave function (27) probably does not take adequate account of the polarization of the hydrogen atom in the field of the incident electron. In order to do this more accurately we shall modify our trial function by making it depend explicitly on r_{12} , the interelectronic distance. Such a wave function can be written as

$$(33) \quad \Psi_t = (1 + c_1 r_{12}) \Phi + \chi ,$$

where $c_1 = 0.31214$ and is the value found by Chandrasekhar. The values of α and β for this wave function are $\alpha = 1.07478$ and $\beta = 0.47758$.

The quantities c , β , and c_1 will again be taken as constants for this calculation.

The integrals involved in the determination of a_0 , b_0 in (28) become somewhat more complicated due to the explicit dependence of the trial function on r_{12} . Their evaluation, however, is still fairly straightforward (see Appendix II).

It should be pointed out here that the antisymmetric form of equations (27) and (33) probably is not a very good trial function for the triplet scattering. In choosing the singlet trial function we were guided in our choice by the fact that a bound state of H^- exists. For the triplet scattering we have no such guide. There is therefore no reason to believe that antisymmetrizing the singlet trial function will lead to a good trial function of the triplet scattering when the electrons are close together.

We shall show in Section 4 that the singlet scattering gives the main contribution to the cross section, so that errors in the triplet trial wave function will make very little difference.

We have therefore not calculated X_0 for the triplet scattering using (33). Furthermore, Massey and Moiseiwitsch indicate in [19] that the polarization correction does not affect the triplet scattering to any great extent.

The results of the aforementioned calculation are given in Table II:

Table II

	X_0	γ	A	B
Singlet	-0.1291	0.07	0.0308	-0.1472

The total cross section Q is given by

$$(34) \quad Q = \frac{1}{4} Q_s + \frac{3}{4} Q_t ,$$

where Q_s and Q_t are the singlet and triplet cross section respectively.

At zero incident electron energy we have

$$(35) \quad \begin{cases} Q_s = 4\pi \lim_{k \rightarrow 0} \left(\frac{\tan^2 \delta_s}{k^2} \right) = 4\pi a_s^2 \\ Q_t = 4\pi \lim_{k \rightarrow 0} \left(\frac{\tan^2 \delta_t}{k^2} \right) = 4\pi a_t^2 . \end{cases}$$

The quantities a_s and a_t are called the scattering lengths and are defined by the relation

$$(36) \quad \lim_{k \rightarrow 0} (k \cot \delta) = -\frac{1}{a} .$$

Using the data of Tables I and II one can easily calculate the total cross section at zero incident electron energy. The results are given in Table III:

Table III

	$\frac{1}{4} Q_s$	$\frac{3}{4} Q_t$	Q
Without Polarization	$66.54 \pi a_0^2$	$16.61 \pi a_0^2$	$83.15 \pi a_0^2$
With Polarization	$60.00 \pi a_0^2$	$16.61 \pi a_0^2$	$76.61 \pi a_0^2$

From Table III it may be seen that the triplet scattering accounts for only about 20% of the total cross section at zero energy. Thus, the singlet scattering is the dominant factor for the process. We also note that the inclusion of the r_{12}^- dependence in the trial wave function lowers the total cross section by about 10%.

3. Dependence of the scattering on the energy of the incident electron

A. Effective range theory. It can be shown for two-body scattering at low energy that the phase shift is given by the relation [2], [3]

$$(37) \quad X = k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 k^2$$

where a is the scattering length and r_0 is called the effective range. The above result is often called the shape-independent formula.

We shall now show that (37) is true for the case of three-body scattering.

We consider the wave equation for a particle of wave number k incident on a two-body system and the wave equation for a zero-energy particle incident on the same two-body system. They can be written in the form

$$(38) \quad \left[\nabla_1^2 + \nabla_2^2 - W + (-B + k^2) \right] \Psi = 0 ,$$

$$(39) \quad \left[\nabla_1^2 + \nabla_2^2 - W - B \right] \Psi_0 = 0 ,$$

where
$$W = \frac{2m}{\hbar^2} V \quad \text{and} \quad B = \frac{2m}{\hbar^2} |E_B| ;$$

where E_B is the binding energy of the two-body system.

We also consider the asymptotic forms of the wave equations (38) and

(39):

$$(40) \quad \left[\nabla_1^2 + \nabla_2^2 + k^2 - B \right] \Phi = 0 ,$$

$$(41) \quad \left[\nabla_1^2 + \nabla_2^2 - B \right] \Phi_0 = 0 .$$

The solutions of equations (40) and (41) can be written as

$$(42) \quad \Phi = \frac{1}{\sqrt{8\pi}} \left[\frac{\sin(kr_1 + \delta)}{r_1 \sin \delta} \phi_n(r_2) \pm \frac{\sin(kr_2 + \delta)}{r_2 \sin \delta} \phi_n(r_1) \right],$$

$$(43) \quad \Phi_0 = \frac{1}{\sqrt{8\pi}} \left[\frac{1}{r_1} \left(1 - \frac{r_1}{a}\right) \phi_n(r_2) \pm \frac{1}{r_2} \left(1 - \frac{r_2}{a}\right) \phi_n(r_1) \right],$$

where $\phi_n(r)$ is the normalized wave function of the two-particle system. The wave function Ψ and Ψ_0 must be well-behaved at the origin, viz:

$$\lim_{r \rightarrow 0} \Psi < \infty \quad \text{and} \quad \lim_{r \rightarrow 0} [r^2 \nabla \Psi] = 0.$$

If we now multiply (38) by Ψ_0 and (39) by Ψ and subtract we obtain

$$(44) \quad \Psi_0 (\nabla_1^2 + \nabla_2^2) \Psi - \Psi (\nabla_1^2 + \nabla_2^2) \Psi_0 + k^2 \Psi \Psi_0 = 0.$$

Similarly from equations (42) and (43) we get

$$(45) \quad \Phi_0 (\nabla_1^2 + \nabla_2^2) \Phi - \Phi (\nabla_1^2 + \nabla_2^2) \Phi_0 + k^2 \Phi \Phi_0 = 0.$$

We now subtract (44) from (45) and integrate over \vec{r}_1 and \vec{r}_2 and apply Green's theorem. We obtain after rearranging terms

$$(46) \quad \begin{aligned} & - \int d\tau_2 \left[\int dS_1 [\Psi_0 \nabla_1 \Psi - \Psi \nabla_1 \Psi_0] + \int dS_1' [\Psi_0 \nabla_1 \Psi - \Psi \nabla_1 \Psi_0] \right] \\ & - \int d\tau_1 \left[\int dS_2 [\Psi_0 \nabla_2 \Psi - \Psi \nabla_2 \Psi_0] + \int dS_2' [\Psi_0 \nabla_2 \Psi - \Psi \nabla_2 \Psi_0] \right] \\ & + \int d\tau_2 \left[\int dS_1 [\Phi_0 \nabla_1 \Phi - \Phi \nabla_1 \Phi_0] + \int dS_1' [\Phi_0 \nabla_1 \Phi - \Phi \nabla_1 \Phi_0] \right] \\ & + \int d\tau_1 \left[\int dS_2 [\Phi_0 \nabla_2 \Phi - \Phi \nabla_2 \Phi_0] + \int dS_2' [\Phi_0 \nabla_2 \Phi - \Phi \nabla_2 \Phi_0] \right] \\ & + k^2 \int d\tau_1 d\tau_2 [\Phi \Phi_0 - \Psi \Psi_0] = 0, \end{aligned}$$

where S' is a large sphere and S is a small sphere near the origin (see Figure 2), both with centers at the origin.

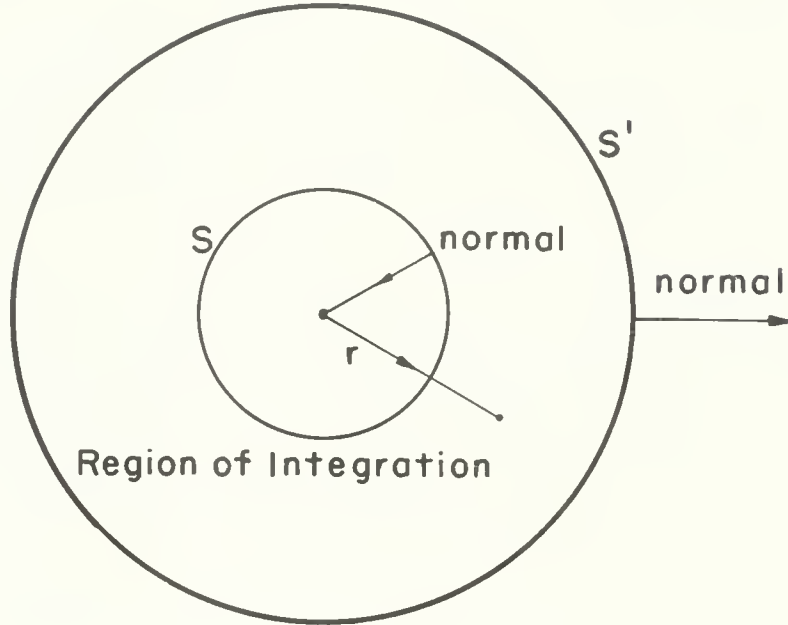


Figure 2

As we let \vec{r} become very large, $\Psi \rightarrow \bar{\Phi}$ and $\Psi_0 \rightarrow \bar{\Phi}_0$, so that the integrals over the large sphere cancel. Furthermore if we let the radius of the small sphere approach zero the integrals of Ψ and Ψ_0 also approach zero because of the conditions imposed on Ψ and $\nabla\Psi$ at the origin. Equation (46) thus reduces to

$$\begin{aligned}
 (47) \quad & \lim_{r_1 \rightarrow 0} \int d\tau_2 \int dS_1 [\bar{\Phi}_0 \nabla_1 \bar{\Phi} - \bar{\Phi} \nabla_1 \bar{\Phi}_0] + \lim_{r_2 \rightarrow 0} \int d\tau_1 dS_2 [\bar{\Phi}_0 \nabla_2 \bar{\Phi} - \bar{\Phi} \nabla_2 \bar{\Phi}_0] \\
 & + k^2 \int d\tau_1 d\tau_2 [\bar{\Phi} \bar{\Phi}_0 - \Psi \Psi_0] = 0 .
 \end{aligned}$$

If we substitute equations (42) and (43) into (47) and carry out the integrations we obtain

$$(48) \quad -k \cot \delta - \frac{1}{a} + k^2 \int d\tau_1 d\tau_2 \left[\bar{\Phi} \Phi_0 - \bar{\Psi} \Psi_0 \right] = 0 .$$

We can expand the wave functions Ψ and $\bar{\Phi}$ as functions of the wave number k :

$$(49) \quad \Psi = \Psi_0 + \Psi_1 k + \Psi_2 k^2 + \dots ,$$

$$(50) \quad \bar{\Phi} = \bar{\Phi}_0 + \bar{\Phi}_1 k + \bar{\Phi}_2 k^2 + \dots ,$$

so that (48) can be written to order k^2 as

$$(51) \quad k \cot \delta = -\frac{1}{a} + k^2 \int d\tau_1 d\tau_2 \left[\bar{\Phi}_0^2 - \Psi_0^2 \right] .$$

If we define the effective range r_0 as

$$(52) \quad \frac{1}{2} r_0 = \int d\tau_1 d\tau_2 \left[\bar{\Phi}_0^2 - \Psi_0^2 \right] ,$$

then (51) becomes

$$(53) \quad k \cot \delta = -\frac{1}{a} + \frac{1}{2} r_0 k^2 ,$$

which is the effective range formula.

If we are dealing with a bound state of the three-particle system we can use the same arguments as were used in obtaining (53), except that the asymptotic wave function $\bar{\Phi}$ must now vanish for very large r . The result of carrying out this argument is to obtain a relation between the attachment energy $\frac{\epsilon^2}{2}$ for the third particle, the scattering length, and the effective range; this relation is

$$(54) \quad \epsilon = \frac{1}{a} + \frac{1}{2} r_0 \epsilon^2 .$$

For S-wave scattering the cross section can be written as

$$(55) \quad Q = \frac{4\pi}{k^2} \sin^2 \delta .$$

For low energies we can use (53), so that (55) becomes

$$(56) \quad Q = \frac{4\pi}{k^2 + k^2 \cot^2 \delta} = \frac{4\pi}{k^2 + \left[-\frac{1}{a} + \frac{1}{2} r_o k^2 \right]^2} .$$

We can thus see that the total cross section (singlet plus triplet) is determined by the four parameters a_s , r_{os} , a_t and r_{ot} .

We have already calculated a_{os} and a_{ot} . Equation (56) is valid so long as $(r_o k)^2$ is negligible compared to $(r_o k)$. We shall see that the limit of applicability is determined by r_{os} . For our problem we can use (56) for values of k up to 0.04 or about 0.02 ev. This is of the order of thermal energy

We now seek a method of calculating r_{os} and r_{ot} . Since a bound state (singlet state) exists for the H^- ion we can use (54) to find r_{os} if we know the attachment energy of the second electron. This quantity has been calculated by Chandrasekhar (result: 0.7019 volts) and measured by Branscomb^[7] (result 0.756 volts). For the triplet scattering no corresponding bound state exists, so that we shall have to use other means to determine r_{ot} .

Returning now to the calculation of r_{os} , we shall use the experimental value of the wave number of the second electron, which is $\epsilon = 0.236$. Substituting this value of ϵ and the values of a_s into (54) we find the results shown in Table IV:

Table IV

	r_{os} (without polarization)	r_{os} (with polarization)
r_{os}	$4.04 a_o$	$3.85 a_o$

B. Independent Calculation of r_0 . The quantity r_{ot} must be evaluated by a method independent of the effective range theory since, as mentioned above, no triplet bound state of H^- exists. If we choose a trial function which depends on the energy of the incident electron, then (25) and (28) will give $X = k \cot \delta$ as a function of the energy of the incident electron. In (28) the quantities a, b, \dots and A and B will also depend upon the energy of the incident electron.

For electrons whose energies are close to zero, we can expand each term in (28) in powers of k . According to (53), we obtain

$$(57) \quad X = p_0 + p_1 k^2 + O(k^3) \quad .$$

Differentiating X with respect to k^2 , we have

$$(58) \quad \frac{\partial X}{\partial k^2} = p_1 + O(k) \quad .$$

In the limit $k \rightarrow 0$, we have, using (37),

$$(59) \quad \lim_{k \rightarrow 0} \left(\frac{\partial X}{\partial k^2} \right) = p_1 = \frac{1}{2} r_0 \quad .$$

We now choose an energy-dependent trial function having the correct asymptotic form, namely

$$(60) \quad \begin{aligned} \psi_t = & A \left[e^{-cr_1} e^{-\beta r_2} + e^{-\beta r_1} e^{-ar_2} \right] \\ & + \frac{1}{\sqrt{8\pi}} \left[\frac{B(1-e^{-\gamma r_1})}{k r_1} \sin k r_1 + \frac{(1-e^{-\gamma r_1})^2}{r_1} \cos k r_1 \right] e^{-r_2} \quad r_1 \rightleftharpoons r_2 \end{aligned}$$

Then equation (25) can be written as

$$(61) \quad X = - \left[aA^2 + bB^2 + cAB + d + eA + (f-1)B \right] .$$

Let us now find $\partial X / \partial k^2$. We have

$$(62) \quad - \frac{\partial X}{\partial k^2} = \frac{\partial a}{\partial k^2} A^2 + \frac{\partial b}{\partial k^2} B^2 + \frac{\partial c}{\partial k^2} AB + \frac{\partial d}{\partial k^2} + \frac{\partial e}{\partial k^2} A + \frac{\partial f}{\partial k^2} B \\ + 2aA \frac{\partial A}{\partial k^2} + 2bB \frac{\partial B}{\partial k^2} + c \left(A \frac{\partial B}{\partial k^2} + B \frac{\partial A}{\partial k^2} \right) + e \frac{\partial A}{\partial k^2} + (f-1) \frac{\partial B}{\partial k^2} .$$

Let

$$(63) \quad a = a_0 + a_1 k^2 + a_2 k^4 + \dots, \quad b = b_0 + b_1 k^2 + b_2 k^4 + \dots, \quad \text{etc.}$$

so that as $k \rightarrow 0$, equation (62) becomes

$$(64) \quad \lim_{k \rightarrow 0} \left(- \frac{\partial X}{\partial k^2} \right) = a_1 A_0^2 + b_1 B_0^2 + c_1 A_0 B_0 + d_1 + e_1 A_0 + f_1 B_0 \\ + \left[2a_0 A_0 + c_0 B_0 + e_0 \right] \left(\frac{\partial A}{\partial k^2} \right)_0 + \left[2b_0 B_0 + c_0 A_0 + (f_0 - 1) \right] \left(\frac{\partial B}{\partial k^2} \right)_0 .$$

From the conditions (29) and (30) we see that the last two terms in (64) vanish, so that we obtain

$$(65) \quad \lim_{k \rightarrow 0} \left(\frac{\partial X}{\partial k^2} \right) = \frac{1}{2} r_0 = - \left[a_1 A_0^2 + b_1 B_0^2 + c_1 A_0 B_0 + d_1 + e_1 A_0 + f_1 B_0 \right] .$$

In the numerical calculation of $\lim_{k \rightarrow 0} \left(\frac{\partial X}{\partial k^2} \right)$ we shall use the value of γ which gave us an extremum for X_0 . This assumption may be justified by the following argument. We may write

$$(66) \quad X = f(A, B, \gamma) + g(A, B, \gamma) k^2 ,$$

where A , B , and γ are functions of k .

Then

$$(67) \quad \left\{ \begin{aligned} \frac{\partial X}{\partial k^2} &= \frac{\partial f}{\partial k^2} + g(A, B, \gamma) + \frac{\partial g}{\partial k^2} k^2 \\ &= \frac{\partial f}{\partial A} \frac{\partial A}{\partial k^2} + \frac{\partial f}{\partial B} \frac{\partial B}{\partial k^2} + \frac{\partial f}{\partial \gamma} \frac{\partial \gamma}{\partial k^2} + g(A, B, \gamma) + \frac{\partial g}{\partial k^2} k^2 \end{aligned} \right.$$

Letting $k \rightarrow 0$ gives

$$(68) \quad \lim_{k \rightarrow 0} \left(\frac{\partial X}{\partial k^2} \right) = \left(\frac{\partial f}{\partial A} \right)_o \left(\frac{\partial A}{\partial k^2} \right) + \left(\frac{\partial f}{\partial B} \right)_o \left(\frac{\partial B}{\partial k^2} \right) + \left(\frac{\partial f}{\partial \gamma} \right)_o \left(\frac{\partial \gamma}{\partial k^2} \right) + g(A_o, B_o, \gamma_o) ,$$

where the subscript o indicates the values $A = A_o$, $B = B_o$ and $\gamma = \gamma_o$, for $k = 0$.

From the fact that X_o is an extremum for $A = A_o$, $B = B_o$ and $\gamma = \gamma_o$ it follows that

$$(69) \quad \left(\frac{\partial f}{\partial A} \right)_o = \left(\frac{\partial f}{\partial B} \right)_o = \left(\frac{\partial f}{\partial \gamma} \right)_o = 0$$

so that (68) reduces to

$$(70) \quad \lim_{k \rightarrow 0} \left(\frac{\partial X}{\partial k^2} \right) = g(A_o, B_o, \gamma_o) = p_1 = \frac{1}{2} r_o .$$

All of the integrals involved can be evaluated by elementary methods (see Appendix III).

The results are shown in Table V:

	<u>Table V</u>	
	Singlet	Triplet
r_o	3.11 a_o	0.808 a_o

The above value of r_{os} differs from that calculated using the effective range theory by about 30%. The present value for r_{os} is probably not as accurate as the one obtained from the effective range theory since the trial function was not as accurate.

In Section 4 we shall discuss the sensitivity of the cross section to the parameters a_s , r_{os} , a_t and r_{ot} . We shall show there that the low-energy cross section is not appreciably influenced by errors in r_{ot} . Hence the above method for calculating r_{ot} need not be discarded because of its inaccuracy.

For the singlet cross section we shall use the value of r_{os} and a_s calculated using the polarization approximation. For the triplet cross section we shall use the value of a_t calculated for the non-polarization approximation, and the value of r_{ot} found from the energy-dependent trial function.

The results of this calculation are given in Table VI:

Table VI

k	$Q_s/\pi a_o^2$	$Q_t/\pi a_o^2$	$\frac{1}{4} Q_s/\pi a_o^2$	$\frac{3}{4} Q_t/\pi a_o^2$	$Q/\pi a_o^2$
0.000	240.0	22.14	60.00	16.61	76.61
0.005	240.0	22.14	60.00	16.61	76.61
0.010	239.2	22.12	59.81	16.59	76.40
0.015	238.2	22.11	59.56	16.58	76.14
0.020	237.2	22.10	59.31	16.58	75.80
0.025	235.4	22.08	58.56	16.56	75.42
0.030	233.5	22.05	58.38	16.54	74.92
0.035	231.1	22.02	57.77	16.52	74.29
0.040	228.6	21.96	57.14	16.47	73.61

These results are plotted on Graph I.

4. Sensitivity of the method

For three-body collisions there is no rigorous way of estimating upper and lower bounds for the phase shifts, so that we have no means of determining the accuracy of our calculation.

We shall, however, determine the effect which errors in a and r_o have upon the cross section for the scattering process.

The total cross section as given by equation (34) is

$$(34) \quad Q = \frac{1}{4} Q_s + \frac{3}{4} Q_t .$$

Suppose there is an error ΔQ_s and ΔQ_t in the values of Q_s and Q_t respectively; then Q will be changed by an amount ΔQ . The relative error $\frac{\Delta Q}{Q}$ is then given by the relation

$$(71) \quad \frac{\Delta Q}{Q} = \frac{\frac{1}{4} Q_s \frac{\Delta Q_s}{Q_s} + \frac{3}{4} Q_t \frac{\Delta Q_t}{Q_t}}{Q} .$$

It can now be shown that an error $\frac{\Delta a}{a}$ in a and $\frac{\Delta r_o}{r_o}$ in r_o leads to an error $\frac{\Delta Q}{Q}$ in Q for either Q_s or Q_t ; this is given by

$$(72) \quad \frac{\Delta Q}{Q} = \frac{k^2 + X^2}{k^2 + \left[-\frac{1}{a(1 + \frac{\Delta a}{a})} + \frac{1}{2} r_o k^2 \left(1 + \frac{\Delta r_o}{r_o} \right) \right]^2} - 1 .$$

For $k = 0$ equation (72) becomes

$$(73) \quad \frac{\Delta Q}{Q} = 2 \frac{\Delta a}{a} + \left(\frac{\Delta a}{a} \right)^2 .$$

We make the supposition that the trial function for the singlet scattering is a good one so that the value of a_s and r_{os} which we have calculated are quite accurate.

For the triplet scattering such accuracy is very unlikely, as pointed out previously. We shall therefore assume that any error in the cross section is due to errors in a_t and r_{ot} .

Before proceeding to examine the effects that errors in a_t and r_{ot} produce in the cross section let us compare our results for zero-energy scattering with those obtained by extrapolating the calculations of Massey and Moiseiwitsch^[19] to zero energy. We shall use the values for what the above authors call the 'exchange-polarization approximation.'

We carry out the extrapolation by plotting $k \cot \delta$ against k^2 (see Graph II). For both the singlet and the triplet case the points fall almost on a straight line. The results obtained from this graph are shown, along with our results, in Table VII:

Table VII

	$k \cot \delta$		r_o	
	M and M	Our Value	M and M	Our Value
Singlet	-0.145	-0.1291	2.67 a_o	3.85 a_o
Triplet	-0.43	-0.4251	1.56 a_o	0.808 a_o

Our values for r_{os} and r_{ot} differ quite markedly from those of Massey and Moiseiwitsch. The values of r_o obtained by extrapolation and by calculating $\lim_{k \rightarrow 0} (\partial X / \partial k^2)$ are probably not as good as those obtained from the effective range formula, since the former method does not insure that a good value of the intercept will yield a good value for the slope of the line, while the latter method is founded on strong theoretical grounds.

Moreover, it can be seen from (72) that the cross section is insensitive to r_0 for small values of k^2 , so that even relatively large errors in r_0 will not have an appreciable effect on the cross section.

Our value for a_s differs from the value obtained by extrapolation from the results of Massey and Moiseiwitsch by about 15% and should be regarded as an improvement due to the use of our more accurate trial function. The values for a_t are about the same for both calculations.

The zero-energy cross section obtained by extrapolation from the Massey and Moiseiwitsch results is $64.6 \pi a_0^2$, as compared to our value of $76.61 \pi a_0^2$, which is about 20% higher. No experiments have been done in the energy range where our calculations are valid, so that there is no way of comparing our calculation of the cross section with experiment. Recent experiments [1] in the region between two and ten volts give values of the cross section higher than those calculated by Massey and Moiseiwitsch for these energies. It thus appears likely that our larger zero-energy cross section is an improvement over the extrapolated calculation of Massey and Moiseiwitsch.

Let us now examine the effect of errors in a_t and r_{ot} on the calculated value of the cross section. As mentioned above, we take the point of view that a_s and r_{os} are accurately known and that a_t and r_{ot} may be in error.

Let us assume that there are large errors in both a_t and r_{ot} . We shall, for the sake of argument, take $\frac{\Delta a_t}{a_t} = 0.50$ and $\frac{\Delta r_{ot}}{r_{ot}} = 1.00$. If we now substitute these values in (72) and apply (71) we obtain the following values for the relative error in the cross section produced by the errors in a_t and r_{ot} :

Table VIII

k	$\frac{\Delta Q}{Q}$ (relative)	$\frac{\Delta Q}{Q}$ (percentage)
0.000	$\frac{20.78}{76.61}$	27.1
0.005	$\frac{20.75}{76.61}$	27.0
0.010	$\frac{20.73}{76.40}$	27.1
0.015	$\frac{20.68}{76.14}$	27.2
0.020	$\frac{20.66}{75.80}$	27.3
0.025	$\frac{20.58}{75.42}$	27.4
0.030	$\frac{20.51}{74.92}$	27.5
0.035	$\frac{20.42}{74.29}$	27.6
0.040	$\frac{20.29}{73.61}$	27.7

From Table VIII we see that the assumed errors in a_t and r_{ot} produce errors in the cross section which are less than 30%. These results are shown on Graph III. If the errors in a_t and r_{ot} are no larger than we have supposed, then the true cross section will lie between curves A and B on Graph III.

Until more rigorous methods are obtained for estimating the errors in this type of calculation the above estimate will have to suffice.

5. Neutral impurity scattering in semiconductors

Measurement of the electrical properties of germanium by Lark-Horowitz and Johnson^[16] and silicon by Pearson and Bardeen^[21] show that the temperature dependence of the resistivity of these materials can not be explained by lattice scattering alone, especially at low temperature. In order to account for the resistivity, the effect of scattering by ionized and neutral impurities must be considered.

Conwell and Weisskopf^[10] have calculated the effect of ionized impurity scattering using the Born approximation, and Erginsoy^[11], using the results of Massey and Moiseiwitsch^[18], has calculated the effect of neutral impurity scattering.

The scattering of holes, or electrons, by neutral impurities in semiconductors is similar to the scattering of electrons by hydrogen atoms. In a semiconductor the radius of the first Bohr orbit of the electron, or the hole, is increased by a factor D , the effective dielectric constant of the material. This would lead to an increase in the cross section by a factor of D^2 .

We shall now obtain an expression for the resistivity as a function of the cross section.

The resistivity can be written as

$$(74) \quad \rho_n = \frac{m}{ne^2\tau},$$

where m is the effective mass of the conduction electron or hole, e is the charge on the conduction electron, n is the concentration of conduction electrons or holes. τ is called the relaxation or collision time and is related to the cross section by

$$(75) \quad \frac{1}{\tau} = \frac{N_n k^2 Q}{m},$$

where N_n is the concentration of neutral impurities in the semiconductor. Combining equations (74) and (75) gives as our expression for ρ_n

$$(77) \quad \rho_n = \frac{kTQ}{e^2} \frac{N_n}{n} \text{ c.g.s.}$$

$$= 3.65 \times 10^{-3} kQ \frac{N_n}{n} \text{ ohm-cm} ,$$

where k and Q are in atomic units, and $D = 13$.

We have calculated ρ_n for silicon-boron, sample 2 and, silicon-phosphorous, sample B, which were investigated by Pearson and Bardeen^[21]. The results are shown and compared with those of Erginsoy in Tables X and XI.

Table X

ρ_n (Silicon-Boron, Sample 2)

		Erginsoy		
$1/T$ ($^{\circ}K$) ⁻¹	ρ_n (ohm-cm)	$1/T$ ($^{\circ}K$) ⁻¹	ρ_n (ohm-cm)	ρ_i (ohm-cm)
0.01018	0.0521	0.012	0.0866	0.0526
0.007072	0.0177	0.010	0.0402	0.0390
0.005198	0.00725	0.006	0.0086	0.0194
0.003978	0.00464	0.005	0.0046	0.0153

Table XI

ρ_n (Silicon-Phosphorous, Sample B)

		Erginsoy		
$1/T$ ($^{\circ}K$) ⁻¹	ρ_n (ohm-cm)	$1/T$ ($^{\circ}K$) ⁻¹	ρ_n (ohm-cm)	ρ_i (ohm-cm)
0.01018	0.0103	0.012	0.0077	0.0283
0.007072	0.00862	0.010	0.0077	0.0250
0.005198	0.00481	0.006	0.0039	0.0155
0.003978	0.00242	0.005	0.0029	0.0129

ρ_i is the resistivity due to scattering by ionized impurities.

The results are also shown on Graphs IV and V.

Our results for the resistivity are larger than those found by Erginsoy, which is to be expected since our values for the cross section are larger than those of Massey and Moiseiwitsch.

These results indicate that the effect of neutral impurity scattering in semiconductors is of more importance than had previously been thought. This is especially true at very low temperatures where the effect of lattice scattering is negligible.

Appendix I. Calculation of variational parameters using $\Psi_t = \Phi + \chi$

We consider the integral

$$\int \Psi_t^L \Psi_t d\tau_1 d\tau_2 ,$$

where Ψ_t is given by equation (27) and L is

$$(I.1) \quad L = v_1^2 + v_2^2 + 2\left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} - \frac{1}{2}\right) .$$

The terms a_0 , b_0 , etc. in (6) are then obtained by evaluating the following integrals:

$$a_0 = \int \left[e^{-ar_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-ar_2} \right] \times L \left[e^{-ar_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-ar_2} \right] d\tau_1 d\tau_2 ;$$

$$b_0 = \frac{1}{8\pi^2} \int \left[(1-e^{-\gamma r_1})e^{-r_2} \pm (1-e^{-\gamma r_2})e^{-r_1} \right] \\ \times L \left[(1-e^{-\gamma r_1})e^{-r_2} \pm (1-e^{-\gamma r_2})e^{-r_1} \right] d\tau_1 d\tau_2 ;$$

$$c_0 = \frac{1}{\sqrt{8}\pi} \left[\int \left[e^{-ar_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-ar_2} \right] \right. \\ \times L \left[(1-e^{-\gamma r_1})e^{-r_2} \pm (1-e^{-\gamma r_2})e^{-r_1} \right] d\tau_1 d\tau_2 \\ \left. + \int \left[(1-e^{-\gamma r_1})e^{-r_2} \pm (1-e^{-\gamma r_2})e^{-r_1} \right] \right. \\ \times L \left[e^{-ar_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-ar_2} \right] d\tau_1 d\tau_2 \left. \right] ;$$

$$d_0 = \frac{1}{8\pi^2} \int \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} + \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] \\ \times L \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} \pm \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] d\tau_1 d\tau_2 ;$$

$$e_o = \frac{1}{\sqrt{8} \pi} \left[\int \left[e^{-\alpha r_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-\alpha r_2} \right] \right. \\ \left. L \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} \pm \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] d\gamma_1 d\gamma_2 \right. \\ \left. + \int \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} \pm \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] \right. \\ \left. L \left[e^{-\alpha r_1} e^{-\beta r_2} \pm e^{-\beta r_1} e^{-\alpha r_2} \right] d\gamma_1 d\gamma_2 \right] ;$$

$$f_o = \frac{1}{8\pi^2} \left[\int \left[(1-e^{-\gamma r_1}) e^{-r_2} \pm (1-e^{-\gamma r_2}) e^{-r_1} \right] \right. \\ \left. L \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} \pm \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] d\gamma_1 d\gamma_2 \right. \\ \left. + \int \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1} \pm \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2} \right] \right. \\ \left. L \left[(1-e^{-\gamma r_1}) e^{-r_2} \pm (1-e^{-\gamma r_2}) e^{-r_1} \right] d\gamma_1 d\gamma_2 \right] .$$

In order to carry out the above integrations we must find the effect of L on the functions upon which it operates. The results of operating with L are listed below:

$$L \left[e^{-\alpha r_1} e^{-\beta r_2} \right] = \left[\alpha^2 + \beta^2 - 1 + \frac{2(1-\alpha)}{r_1} + \frac{2(1-\beta)}{r_2} - \frac{2}{r_{12}} \right] e^{-\alpha r_1} e^{-\beta r_2} ;$$

$$L \left[e^{-\beta r_1} e^{-\alpha r_2} \right] = \left[\alpha^2 + \beta^2 - 1 + \frac{2(1-\beta)}{r_1} + \frac{2(1-\alpha)}{r_2} - \frac{2}{r_{12}} \right] e^{-\beta r_1} e^{-\alpha r_2} ;$$

$$L\left[(1-e^{-\gamma r_1})e^{-r_2}\right] = \frac{2\gamma e^{-\gamma r_1} e^{-r_2}}{r_1} - \gamma^2 e^{-\gamma r_1} e^{-r_2} + \left(\frac{2}{r_1} - \frac{2}{r_{12}}\right)(1-e^{-\gamma r_1})e^{-r_2};$$

$$L\left[(1-e^{-\gamma r_2})e^{-r_1}\right] = \frac{2\gamma e^{-\gamma r_2} e^{-r_1}}{r_2} - \gamma^2 e^{-\gamma r_2} e^{-r_1} + \left(\frac{2}{r_2} - \frac{2}{r_{12}}\right)(1-e^{-\gamma r_2})e^{-r_1};$$

$$L\left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1}\right] = \frac{4\gamma^2 e^{-2\gamma r_1} e^{-r_2}}{r_1} - \frac{2\gamma^2 e^{-\gamma r_1} e^{-r_2}}{r_1} + \left(\frac{2}{r_1} - \frac{2}{r_{12}}\right) \frac{(1-e^{-\gamma r_1})^2 e^{-r_2}}{r_1};$$

$$L\left[\frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2}\right] = \frac{4\gamma^2 e^{-2\gamma r_2} e^{-r_1}}{r_2} - \frac{2\gamma^2 e^{-\gamma r_2} e^{-r_1}}{r_2} + \left(\frac{2}{r_2} - \frac{2}{r_{12}}\right) \frac{(1-e^{-\gamma r_2})^2 e^{-r_1}}{r_2}.$$

Using the above relations the integrals can be evaluated by elementary methods. The results of these calculations give for a_0 , b_0 , etc.:

$$a_0 = 32\pi^2 \left[\frac{1}{8a^2\beta^2} \left(\frac{a^2 + \beta^2 - 1}{2a\beta} + \frac{1-a}{\beta} + \frac{1-\beta}{a} - \frac{a^2 + 3a\beta + \beta^2}{(a+\beta)^3} \right) \right. \\ \left. + \frac{1}{(a+\beta)^5} \left(\frac{4(a^2 + \beta^2 - 1)}{a+\beta} - 4(a+\beta) + \frac{11}{2} \right) \right];$$

$$b_0 = 4 \left[\left(\frac{1}{4} - \frac{1}{16\gamma} - \frac{\gamma+4}{(\gamma+2)^3} - \frac{\gamma+2}{8(\gamma+1)^3} \right) + \left(\frac{4\gamma}{(1+\gamma)^2} \left[1 - \frac{1}{(1+\gamma)^3} - \frac{\gamma}{1+\gamma} + \frac{\gamma}{(1+\gamma)^4} \right] \right. \right. \\ \left. \left. + 4 \left[\frac{3}{8} - \frac{\gamma+3}{(\gamma+2)^3} - \frac{2\gamma+3}{(\gamma+1)^3(\gamma+2)^3} + \frac{3(\gamma+1)}{8(\gamma+1)^6} \right] \right) \right];$$

$$c_0 = \frac{128\pi}{\sqrt{2}} \left[\frac{1}{(1+\beta)^3} \left(\frac{a\gamma}{(a+\gamma)^3} + \frac{a+2(1+\beta)}{(a+\beta+1)^3} - \frac{a+\gamma+2(1+\beta)}{(a+\beta+\gamma+1)^3} \right) \right. \\ \left. + \frac{1}{(1+a)^3} \left(\frac{\beta\gamma}{(\beta+\gamma)^3} + \frac{\beta+2(1+a)}{(a+\beta+1)^3} - \frac{\beta+\gamma+2(1+a)}{(a+\beta+\gamma+1)^3} \right) \right];$$

$$d_o^* = 4 \left[\left(2 \log(1 + \frac{\gamma}{2}) - 3 \log(1+\gamma) + 2 \log(1 + \frac{3\gamma}{2}) - \frac{1}{2} \log(1+2\gamma) \right. \right. \\ \left. \left. + \frac{1}{4} - \frac{2}{2+\gamma} + \frac{3}{2(1+\gamma)} - \frac{2}{2+3\gamma} + \frac{1}{4(1+2\gamma)} - \frac{\gamma}{12} \right) \right. \\ \left. + \left(\left[\frac{4\gamma^2}{(1+2\gamma)^2} - \frac{2\gamma^2}{(1+\gamma)^2} \right] \left[1 - \frac{2}{(1+\gamma)^2} + \frac{1}{(1+2\gamma)^2} \right] + 2 \left[\frac{1}{2} - \frac{2}{2+\gamma} + \frac{1}{2(1+\gamma)} \right] \right. \right. \\ \left. \left. - \frac{4}{(1+\gamma)^2} \left[\frac{1}{2+\gamma} - \frac{1}{1+\gamma} + \frac{1}{2+3\gamma} \right] + \frac{2}{(1+2\gamma)^2} \left[\frac{1}{2(1+\gamma)} - \frac{2}{2+3\gamma} + \frac{1}{2(1+2\gamma)} \right] \right) \right];$$

$$e_o = \frac{64\pi}{\gamma^2} \left[\left(\frac{2\gamma^2}{(1+\beta)^3} \left[\frac{2}{(a+2\gamma)^2} - \frac{1}{(a+\gamma)^2} \right] + \frac{1}{(1+\beta)^3} \left[\frac{2a+3(1+\beta)}{(a+\beta+1)^2} \right. \right. \right. \\ \left. \left. - \frac{2[2(a+\gamma)+3(1+\beta)]}{(a+\beta+\gamma+1)^2} + \frac{2(a+2\gamma)+3(1+\beta)}{(a+\beta+2\gamma+1)^2} \right] \right) \\ \left. + \left(\frac{2\gamma^2}{(1+a)^3} \left[\frac{2}{(\beta+2\gamma)^2} - \frac{1}{(\beta+\gamma)^2} \right] + \frac{1}{(1+a)^3} \left[\frac{2\beta+3(1+a)}{(a+\beta+1)^2} \right. \right. \right. \\ \left. \left. - \frac{2[2(\beta+\gamma)+3(1+a)]}{(a+\beta+\gamma+1)^2} + \frac{2(\beta+2\gamma)+3(1+a)}{(a+\beta+2\gamma+1)^2} \right] \right) \right];$$

$$f_o = 4 \left[\left(\frac{19}{36} - \frac{1}{2} \left[\frac{\gamma+3}{(\gamma+2)^2} - \frac{2\gamma+3}{4(\gamma+1)^2} + \frac{\gamma+1}{(3\gamma+2)^2} \right] \right) \right. \\ \left. + 4 \left(\frac{\gamma}{(1+\gamma)^3} \left[1 - \frac{2}{(1+\gamma)^2} + \frac{1}{(1+2\gamma)^2} \right] + \frac{1}{4} - \frac{2}{(1+\gamma)^2(2+\gamma)^2} \right. \right. \\ \left. \left. + \frac{1}{4(1+\gamma)^2(1+2\gamma)^2} - \frac{1}{(2+\gamma)^2} + \frac{1}{2(1+\gamma)^4} - \frac{1}{(1+2\gamma)^2(2+3\gamma)^2} \right) \right].$$

*Natural log.

Appendix II. Calculation of variational parameters using $\Psi_t = (1 + c_1 r_{12}) \Phi + \chi$.

We consider here the evaluation of the integral

$$I = \int \Psi_t L \Psi_t d\tau_1 d\tau_2$$

where Ψ_t is given by

$$(33) \quad \Psi_t = (1 + c_1 r_{12}) \Phi + \chi .$$

We can then write

$$I = P + Q + R + S ,$$

where

$$\begin{aligned} P &= \int (\Phi + \chi) L(\Phi + \chi) d\tau_1 d\tau_2 \\ Q &= \int (\Phi + \chi) L(c_1 r_{12} \Phi) d\tau_1 d\tau_2 \\ R &= \int c_1 r_{12} \Phi L(\Phi + \chi) d\tau_1 d\tau_2 \\ S &= \int c_1 r_{12} \Phi L(c_1 r_{12} \Phi) d\tau_1 d\tau_2 . \end{aligned}$$

P has already been evaluated in Appendix I.

It can then be easily shown by using Green's theorem that $Q = R$.

Since we have already evaluated the quantity $L(\Phi + \chi)$ it will be simpler to use the integral R.

The integral S can be simplified by putting in the explicit value of

L. We can then write

$$S = S_1 + S_2 ,$$

where

$$\begin{aligned} S_1 &= c_1^2 \int r_{12} \Phi (\nabla_1^2 + \nabla_2^2) (r_{12} \Phi) d\tau_1 d\tau_2 , \\ S_2 &= 2c_1^2 \int (r_{12} \Phi)^2 \left(\frac{1}{r_1} + \frac{1}{r_2} - \frac{1}{r_{12}} - \frac{1}{2} \right) d\tau_1 d\tau_2 ; \end{aligned}$$

S_2 can not be simplified any further.

From the symmetry of Φ it is clear that we have $\nabla_1^2 \Phi = \nabla_2^2 \Phi$. S_1 can then be written as

$$S_1 = 2c_1^2 \int r_{12} \Phi \nabla_1^2 (r_{12} \Phi) d\tau_1 d\tau_2.$$

It is then not difficult to show that S_1 takes the form

$$\begin{aligned} S_1 &= -2c_1^2 \int [\nabla_1(r_{12} \Phi)]^2 d\tau_1 d\tau_2 \\ &= -2c_1^2 \int [\Phi^2 + r_{12}^2 (\nabla_1 \Phi)^2 + 2r_{12} \Phi (\nabla r_{12}) \cdot (\nabla_1 \Phi)] d\tau_1 d\tau_2 \end{aligned}$$

where ∇_1 is the usual gradient operator and where we have used the fact the $(\nabla_1 r_{12})^2 = 1$. All of the above integrals can again be evaluated by elementary methods.

The only terms which will be affected by the r_{12} -term are those which depend on α and β ; these are a_0 , c_0 and e_0 .

Below we list the additional terms a'_0 , c'_0 and e'_0 which must be added to those calculated in Appendix I for a_0 , c_0 and e_0 :

$$\begin{aligned} a'_0 &= 32\pi^2 c_1 \left[\left(\frac{\alpha^2 + \beta^2 - 1}{16(\alpha + \beta)^3} \left[\frac{40}{\beta(\alpha + \beta)^3} + \frac{20}{\beta^2(\alpha + \beta)^2} + \frac{9}{\beta^3(\alpha + \beta)} + \frac{3}{\beta^4} + \frac{40}{\alpha(\alpha + \beta)^3} \right. \right. \right. \\ &\quad \left. \left. \left. + \frac{20}{\alpha^2(\alpha + \beta)^2} + \frac{9}{\alpha^3(\alpha + \beta)} + \frac{3}{\alpha^4} \right] \right. \right. \\ &\quad \left. + \frac{(1-\alpha)}{8(\alpha + \beta)^2} \left[\frac{16}{\beta(\alpha + \beta)^3} + \frac{10}{\beta^2(\alpha + \beta)^2} + \frac{6}{\beta^3(\alpha + \beta)} + \frac{3}{\beta^4} + \frac{16}{\alpha(\alpha + \beta)^3} + \frac{6}{\alpha^2(\alpha + \beta)^2} + \frac{2}{\alpha^3(\alpha + \beta)} \right] \right. \\ &\quad \left. + \frac{(1-\beta)}{8(\alpha + \beta)^2} \left[\frac{16}{\alpha(\alpha + \beta)^3} + \frac{10}{\alpha^2(\alpha + \beta)^2} + \frac{6}{\alpha^3(\alpha + \beta)} + \frac{3}{\alpha^4} + \frac{16}{\beta(\alpha + \beta)^3} + \frac{6}{\beta^2(\alpha + \beta)^2} + \frac{2}{\beta^3(\alpha + \beta)} \right] \right. \\ &\quad \left. - \frac{1}{4\alpha^3\beta^3} \right) + \left(\frac{35(\alpha^2 + \beta^2 - 1)}{(\alpha + \beta)^7} + \frac{44 - 30(\alpha - \beta)}{(\alpha + \beta)^6} \right) \Bigg] \end{aligned}$$

$$\begin{aligned}
 & + \frac{8\pi c_1^2}{\gamma^2} \left[\frac{3}{8a^2\beta^3} \left[\frac{1}{a^2} + \frac{2}{\beta^2} \right] + \frac{3}{8a^3\beta^2} \left[\frac{1}{\beta^2} + \frac{2}{a^2} \right] - \frac{1}{8(a+\beta)^3} \left[\frac{40}{\beta(a+\beta)^3} + \frac{20}{\beta^2(a+\beta)^2} + \frac{9}{\beta^3(a+\beta)} + \frac{3}{\beta^4} \right] \right. \\
 & - \frac{1}{8(a+\beta)^3} \left[a \rightleftharpoons \beta \right] - \frac{3}{8a^3\beta^3} \left[\frac{1}{a^2} + \frac{1}{\beta^2} \right] + \frac{218}{(a+\beta)^7} - \frac{96}{(a+\beta)^8} - \frac{1}{2a^3\beta^3} + \frac{16}{(a+\beta)^6} \\
 & \left. - \frac{384a\beta}{(a+\beta)^8} - \frac{3}{4a\beta^3} \left[\frac{1}{a^2} + \frac{1}{\beta^2} \right] - \frac{3}{4a^3\beta} \left[\frac{1}{a^2} + \frac{1}{\beta^2} \right] \right]
 \end{aligned}$$

$$\begin{aligned}
 c'_0 = & \frac{32\pi c_1}{\gamma^2} \left[\left(\frac{8\gamma}{(a+\beta+\gamma+1)^2} \left[\frac{16}{(1+\beta)(a+\beta+\gamma+1)^3} + \frac{10}{(1+\beta)^2(a+\beta+\gamma+1)^2} + \frac{6}{(1+\beta)^3(a+\beta+\gamma+1)} \right. \right. \right. \\
 & \left. \left. + \frac{3}{(1+\beta)^4} + \frac{16}{(a+\gamma)(a+\beta+\gamma+1)^3} + \frac{6}{(a+\gamma)^2(a+\beta+\gamma+1)^2} + \frac{2}{(a+\gamma)^3(a+\beta+\gamma+1)} \right] \right. \\
 & - \frac{8\gamma^2}{(a+\beta+\gamma+1)^3} \left[\frac{40}{(1+\beta)(a+\beta+\gamma+1)^3} + \frac{20}{(1+\beta)^2(a+\beta+\gamma+1)^2} + \frac{9}{(1+\beta)^3(a+\beta+\gamma+1)} \right. \\
 & \left. \left. + \frac{3}{(1+\beta)^4} + \frac{40}{(a+\gamma)(a+\beta+\gamma+1)^3} + \frac{20}{(a+\gamma)^2(a+\beta+\gamma+1)^2} + \frac{9}{(a+\gamma)^3(a+\beta+\gamma+1)} + \frac{3}{(a+\gamma)^4} \right] \right. \\
 & + \frac{8}{(a+\beta+1)^2} \left[\frac{16}{(1+\beta)(a+\beta+1)^3} + \frac{10}{(1+\beta)^2(a+\beta+1)^2} + \frac{6}{(1+\beta)^3(a+\beta+1)} + \frac{3}{(1+\beta)^4} \right. \\
 & \left. \left. + \frac{16}{a(a+\beta+1)^3} + \frac{6}{a^2(a+\beta+1)^2} + \frac{2}{a^3(a+\beta+1)} \right] - \frac{8}{(a+\beta+\gamma+1)} [a \rightarrow a+\gamma] \right. \\
 & \left. - \frac{16}{(1+\beta)^3} \left[\frac{1}{a^3} - \frac{1}{(a+\gamma)^3} \right] \right) + (a \rightleftharpoons \beta) \Bigg] ;
 \end{aligned}$$

$$\begin{aligned}
 e_o^{*,*} = & \frac{32\pi c_1}{\gamma^2} \left[\left(8\gamma^2 \left[\frac{16}{(1+\beta)(\alpha+\beta+2\gamma+1)^5} + \frac{10}{(1+\beta)^2(\alpha+\beta+2\gamma+1)^4} + \frac{6}{(1+\beta)^3(\alpha+\beta+2\gamma+1)^3} \right. \right. \right. \\
 & \left. \left. + \frac{3}{(1+\beta)^4(\alpha+\beta+2\gamma+1)^2} + \frac{16}{(\alpha+2\gamma)(\alpha+\beta+2\gamma+1)^5} + \frac{6}{(\alpha+2\gamma)^2(\alpha+\beta+2\gamma+1)^4} + \frac{2}{(\alpha+2\gamma)^3(\alpha+\beta+2\gamma+1)^3} \right] \right. \\
 & - 4\gamma^2 \left[\text{as above with } (\alpha + 2\gamma) \rightarrow (\alpha + \gamma) \right] \\
 & + 4 \left[\frac{3}{(1+\beta)(\alpha+\beta+1)^4} + \frac{2}{(1+\beta)^2(\alpha+\beta+1)^3} + \frac{1}{(1+\beta)^3(\alpha+\beta+1)^2} - \frac{1}{(1+\beta)^4(\alpha+\beta+1)} \right. \\
 & \left. + \frac{3}{\alpha(\alpha+\beta+1)^4} + \frac{1}{\alpha^2(\alpha+\beta+1)^3} + \frac{4}{(1+\beta)^5} \log \frac{\alpha+\beta+1}{\alpha} \right] \\
 & - 8[\alpha \rightarrow \alpha+\gamma] + 4[\alpha \rightarrow \alpha+2\gamma] - \frac{4}{(1+\beta)^3} \left[\frac{1}{\alpha^2} - \frac{2}{(\alpha+\gamma)^2} + \frac{1}{(\alpha+2\gamma)^2} \right] \Bigg) \\
 & + (\alpha \rightleftharpoons \beta) \Bigg] .
 \end{aligned}$$

*Natural log.

Appendix III. Calculations required for r_{os} and r_{ot} with energy-dependent trial functions

We wish to calculate the quantities a_1 , b_1 , etc. in equation (63).

In order to accomplish this we must evaluate

$$\frac{\partial}{\partial k^2} \int \Psi_t L \Psi_t d\gamma_1 d\gamma_2 ,$$

where Ψ_t is the energy-dependent trial function given in (60) and L is

$$L = \nabla_1^2 + \nabla_2^2 + \left(\frac{2}{r_1} + \frac{2}{r_2} - \frac{2}{r_{12}} - 1 + k^2 \right) .$$

To carry out the calculation we must find the result of operating on the asymptotic part of (63) with L . These results are listed below:

$$\begin{aligned} L \left[\frac{(1-e^{-\gamma r_1}) e^{-r_2} \sin kr_1}{k r_1} \right] &= \left(\frac{2}{r_1} - \frac{2}{r_{12}} \right) \frac{(1-e^{-\gamma r_1}) e^{-r_2} \sin kr_1}{k r_1} \\ &+ \frac{2\gamma e^{-\gamma r_1} e^{-r_2} \cos kr_1}{r_1} - \frac{\gamma^2 e^{-\gamma r_1} e^{-r_2} \sin kr_1}{k r_1} ; \\ L \left[\frac{(1-e^{-\gamma r_1})^2 e^{-r_2} \cos kr_1}{r_1} \right] &= \left(\frac{2}{r_1} - \frac{2}{r_{12}} \right) \frac{(1-e^{-\gamma r_1})^2 e^{-r_2} \cos kr_1}{r_1} \\ &- \frac{4\gamma(1-e^{-\gamma r_1}) e^{-\gamma r_1} e^{-r_2} k \sin kr_1}{r_1} + \frac{4\gamma^2 e^{-2\gamma r_1} e^{-r_2} \cos kr_1}{r_1} - \frac{2\gamma^2 e^{-\gamma r_1} e^{-r_2} \cos kr_1}{r_1} . \end{aligned}$$

The results for r_1 and r_2 interchanged are exactly the same as those above with r_1 and r_2 interchanged.

With these results we can now carry out the calculation of

$$\frac{\partial}{\partial k^2} \int \Psi_t L \Psi_t d\gamma_1 d\gamma_2$$

to terms of order k^2 .

We now list the values of a_1 , b_1 , etc.:

$$a_1 = 32\pi^2 \left[\frac{1}{16\alpha^3 \beta^3} \pm \frac{4}{(\alpha+\beta)^6} \right];$$

$$\begin{aligned} b_1 = & -4 \left[\frac{3}{16} - \frac{4}{(2+\gamma)^4} \left(\frac{2}{2+\gamma} + \frac{1}{2} \right) + \frac{1}{16(1+\gamma)^4} \left(\frac{2}{1+\gamma} + 1 \right) - \frac{1}{16\gamma^3} \right. \\ & + \left(-\frac{4}{(2+\gamma)^2} \left(\frac{2}{(2+\gamma)^3} + \frac{3}{(2+\gamma)^2} + \frac{3}{2+\gamma} + 2 \right) + \frac{5}{(1+\gamma)^7} + 5 \right. \\ & - \frac{4}{(1+\gamma)^2(2+\gamma)^2} \left(\frac{3}{(2+\gamma)^3} + \frac{3}{(1+\gamma)(2+\gamma)^2} + \frac{3}{(1+\gamma)^2(2+\gamma)} + \frac{2}{(1+\gamma)^3} \right) \\ & - \frac{4}{(2+\gamma)^4} \left(\frac{2}{2+\gamma} + 1 \right) - \frac{4}{(1+\gamma)^2(2+\gamma)^4} \left(\frac{2}{2+\gamma} + \frac{1}{1+\gamma} \right) \\ & \left. + \frac{8\gamma}{(1+\gamma)^3} \left(1 - \frac{1}{(1+\gamma)^5} \right) + \left(\frac{128}{(1+\gamma)^4} - \frac{8\gamma^2}{(1+\gamma)^5} \right) \left(1 - \frac{1}{(1+\gamma)^3} \right) \right]; \end{aligned}$$

$$\begin{aligned} c_1 = & -\frac{16\pi}{\sqrt{2}} \left[\frac{4}{(\alpha+\beta+1)} \left(\frac{1}{(1+\beta)^2} \left(\frac{2}{\alpha+\beta+1} + \frac{1}{1+\beta} \right) \pm \frac{1}{(1+\alpha)^2} \left(\frac{2}{\alpha+\beta+1} + \frac{1}{1+\alpha} \right) \right) \right. \\ & + 4\gamma \left(\frac{1}{(\alpha+\gamma)^4(1+\beta)^3} \left(3 - \frac{2\gamma}{\alpha+\gamma} \right) \pm \frac{1}{(\beta+\gamma)^4(1+\alpha)^3} \left(3 - \frac{2\gamma}{\beta+\gamma} \right) \right) \\ & + \frac{4}{(1+\beta)^3} \left(\frac{1}{\alpha^3} - \frac{1}{(\alpha+\gamma)^3} \right) \pm \frac{4}{(1+\alpha)^3} \left(\frac{1}{\beta^3} - \frac{1}{(\beta+\gamma)^3} \right) \\ & \left. + \left(\frac{8\alpha^2}{(1+\beta)^3} \left(\frac{1}{\alpha^5} - \frac{1}{(\alpha+\gamma)^5} \right) + \frac{4(1-\alpha)}{(1+\beta)^3} \left(\frac{1}{\alpha^4} - \frac{1}{(\alpha+\gamma)^4} \right) \right) \right] \end{aligned}$$

$$- \frac{4}{(\alpha+\beta+1)^3} \left(\frac{2}{(1+\beta)^2(\alpha+\beta+1)^2} + \frac{1}{\alpha^3(1+\beta)} + \frac{3}{\alpha^2(1+\beta)(\alpha+\beta+1)} + \frac{6}{\alpha(1+\beta)(\alpha+\beta+1)^2} \right. \\ \left. + \frac{1}{\alpha^4} + \frac{2}{\alpha^3(\alpha+\beta+1)} + \frac{2}{\alpha^2(\alpha+\beta+1)^2} \right) + \frac{4}{(\alpha+\beta+\gamma+1)^3} (\alpha \rightarrow \alpha+\gamma) \pm (\alpha \leftrightarrow \beta) \Bigg];$$

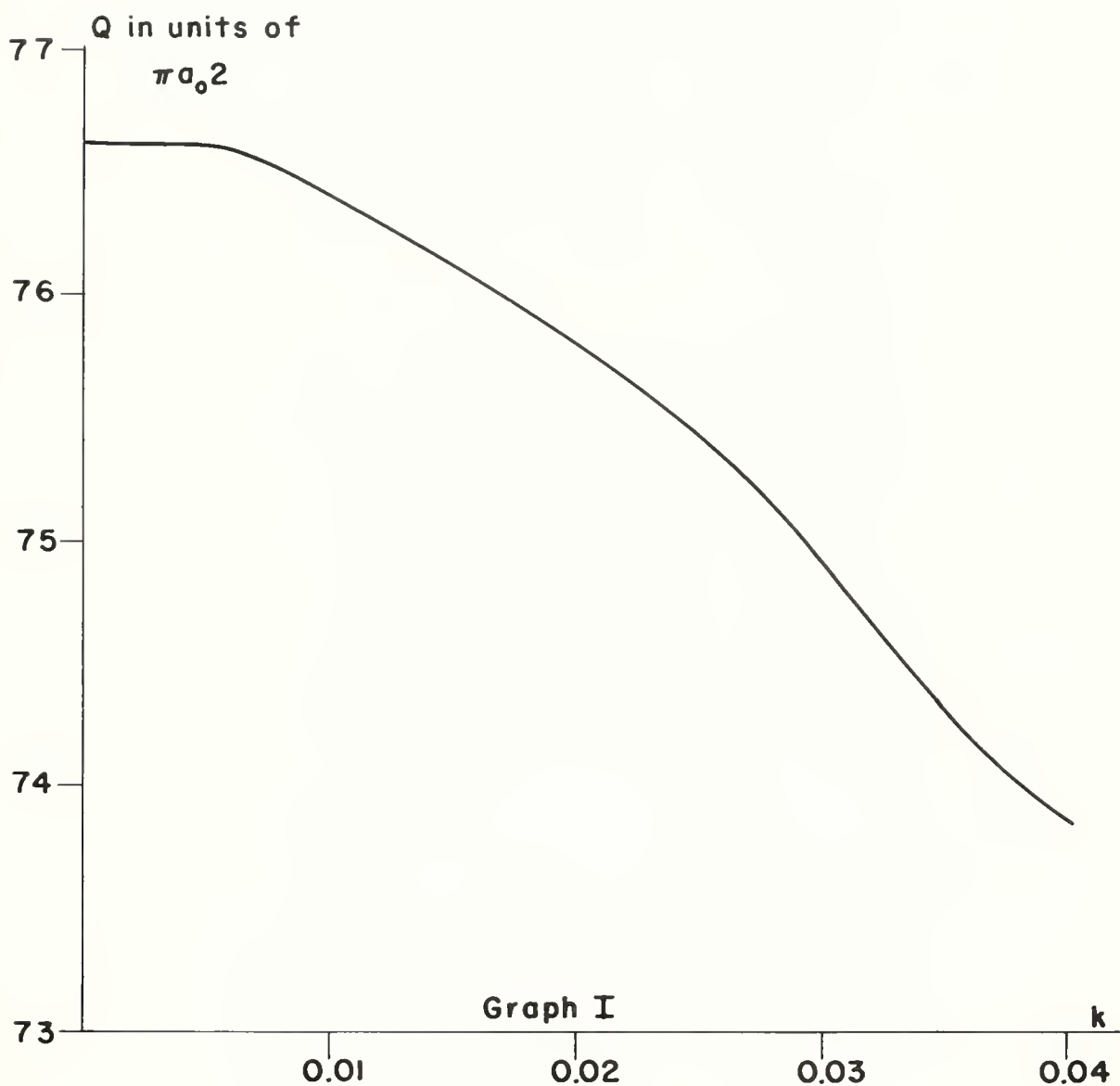
$$d_1 = -4 \left[\frac{1}{4} - \frac{1}{2} \left(\frac{4(\gamma+4)}{(\gamma+2)^3} - \frac{3(\gamma+2)}{2(\gamma+1)^3} + \frac{4(3\gamma+4)}{(3\gamma+2)^3} - \frac{(\gamma+1)}{2(2\gamma+1)^3} \right) - \frac{115}{864\gamma} \pm \left(\frac{9}{2} - \frac{4}{(2+\gamma)^3} \right. \right. \\ \left. + \frac{1}{4(1+\gamma)^3} - \frac{4}{(1+\gamma)^2(2+\gamma)^3} + \frac{1}{(1+\gamma)^5} - \frac{4}{(1+\gamma)^2(2+3\gamma)^3} + \frac{1}{4(1+2\gamma)^2(1+\gamma)^3} \right. \\ \left. - \frac{4}{(1+2\gamma)^2(2+3\gamma)^3} + \frac{1}{4(1+2\gamma)^5} - \frac{4}{(2+\gamma)} \left(\frac{1}{(2+\gamma)^2} + \frac{2}{2+\gamma} + 3 \right) \right. \\ \left. + \frac{1}{(1+\gamma)} \left(\frac{1}{4(1+\gamma)^2} + \frac{1}{1+\gamma} + 3 \right) - \frac{4}{(1+\gamma)^2(2+\gamma)} \left(\frac{1}{(2+\gamma)^2} + \frac{2}{(1+\gamma)(2+\gamma)} + \frac{3}{(1+\gamma)^2} \right) \right. \\ \left. + \frac{17}{(1+\gamma)^5} - \frac{4}{(1+\gamma)^2(2+3\gamma)} \left(\frac{1}{(2+3\gamma)^2} + \frac{2}{(1+\gamma)(2+3\gamma)} + \frac{3}{(1+\gamma)^2} \right) \right. \\ \left. + \frac{1}{(1+2\gamma)^2(1+\gamma)} \left(\frac{1}{4(1+\gamma)^2} + \frac{1}{(1+\gamma)(1+2\gamma)} + \frac{3}{(1+2\gamma)^2} \right) \right. \\ \left. - \frac{4}{(1+2\gamma)^2(2+3\gamma)} \left(\frac{1}{(2+3\gamma)^2} + \frac{2}{(1+2\gamma)(2+3\gamma)} + \frac{3}{(1+2\gamma)^2} \right) + \frac{17}{4(1+2\gamma)^5} \right. \\ \left. + \left(\frac{12\gamma^2}{(1+2\gamma)^4} - \frac{6\gamma^2}{(1+\gamma)^4} \right) \left(1 - \frac{2}{(1+\gamma)^2} + \frac{1}{(1+2\gamma)^2} \right) + \left(\frac{8\gamma}{(1+\gamma)^3} - \frac{8\gamma}{(1+2\gamma)^3} \right) \right. \\ \left. \left(1 - \frac{2}{(1+\gamma)^2} + \frac{1}{(1+2\gamma)^2} \right) + \left(\frac{12\gamma^2}{(1+2\gamma)^2} - \frac{6\gamma^2}{(1+\gamma)^2} \right) \left(1 - \frac{2}{(1+\gamma)^4} + \frac{1}{(1+2\gamma)^4} \right) \right] \Bigg];$$

$$\begin{aligned}
 e_1 = & -\frac{16\pi}{\sqrt{2}} \left[\left(\frac{2}{(1+\beta)^2(\alpha+\beta+1)^3} \left(\frac{3}{\alpha+\beta+1} + \frac{2}{1+\beta} \right) - \frac{4}{(1+\beta)^2(\alpha+\beta+\gamma+1)^3} \left(\frac{3}{\alpha+\beta+\gamma+1} + \frac{2}{1+\beta} \right) \right. \right. \\
 & + \frac{2}{(1+\beta)^2(\alpha+\beta+2\gamma+1)^3} \left(\frac{3}{\alpha+\beta+2\gamma+1} + \frac{2}{1+\beta} \right) + \frac{12\gamma^2}{(1+\beta)^3} \left(\frac{2}{(\alpha+2\gamma)^4} - \frac{1}{(\alpha+\gamma)^4} \right) \\
 & \left. + \frac{16\gamma}{(1+\beta)^3} \left(\frac{1}{(\alpha+\gamma)^3} - \frac{1}{(\alpha+2\gamma)^3} \right) \right) \pm (\alpha \rightleftharpoons \beta) \\
 & + \frac{2}{(1+\beta)^3} \left(\frac{1}{\alpha^2} - \frac{2}{(\alpha+\gamma)^2} + \frac{1}{(\alpha+2\gamma)^2} \right) + \frac{2}{(1+\alpha)^3} \left(\frac{1}{\beta^2} - \frac{2}{(\beta+\gamma)^2} + \frac{1}{(\beta+2\gamma)^2} \right) \\
 & + \left(\frac{6\alpha^2}{(1+\beta)^3} \left(\frac{1}{\alpha^4} - \frac{2}{(\alpha+\gamma)^4} + \frac{1}{(\alpha+2\gamma)^4} \right) + \frac{4(1-\alpha)}{(1+\beta)^3} \left(\frac{1}{\alpha^3} - \frac{2}{(\alpha+\gamma)^3} + \frac{1}{(\alpha+2\gamma)^3} \right) \right. \\
 & - \frac{2}{(\alpha+\beta+1)^3} \left(\frac{3}{(1+\beta)^2(\alpha+\beta+1)} + \frac{3}{\alpha^2(1+\beta)} + \frac{9}{\alpha(1+\beta)(\alpha+\beta+1)} + \frac{2}{\alpha^3} + \frac{3}{\alpha^2(\alpha+\beta+1)} \right) \\
 & \left. + \frac{4}{(\alpha+\beta+\gamma+1)^3} (\alpha \rightarrow \alpha+\gamma) - \frac{2}{(\alpha+\beta+2\gamma+1)} (\alpha \rightarrow \alpha+2\gamma) \right) \pm (\alpha \rightleftharpoons \beta) \Bigg] ;
 \end{aligned}$$

$$\begin{aligned}
 f_1 = & -4 \left[\frac{5}{12} - \frac{1}{8\gamma^2} - \frac{4}{3} \left(\frac{3}{(\gamma+2)^3} \left(\frac{3}{\gamma+2} + 1 \right) - \frac{3}{16(1+\gamma)^3} \left(\frac{3}{1+\gamma} + 2 \right) \right. \right. \\
 & \left. + \frac{1}{(3\gamma+2)^3} \left(\frac{1}{3\gamma+2} + 1 \right) \right) \pm \left(-\frac{4}{(2+\gamma)^3} \left(\frac{3}{2+\gamma} + 2 \right) + \frac{1}{4(1+\gamma)^3} \left(\frac{1}{1+\gamma} + 2 \right) \right. \\
 & - \frac{2}{(1+\gamma)^2(2+\gamma)^3} \left(\frac{3}{2+\gamma} + \frac{2}{1+\gamma} \right) + \frac{7}{4(1+\gamma)^6} - \frac{2}{(1+\gamma)^2(2+3\gamma)^3} \left(\frac{3}{2+3\gamma} + \frac{2}{1+\gamma} \right) \\
 & \left. + \left(\frac{24}{(1+2\gamma)^4} - \frac{16\gamma}{(1+2\gamma)^3} - \frac{12}{(1+\gamma)^4} + \frac{16\gamma}{(1+\gamma)^3} \right) \left(1 - \frac{1}{(1+\gamma)^3} \right) + 10 \right]
 \end{aligned}$$

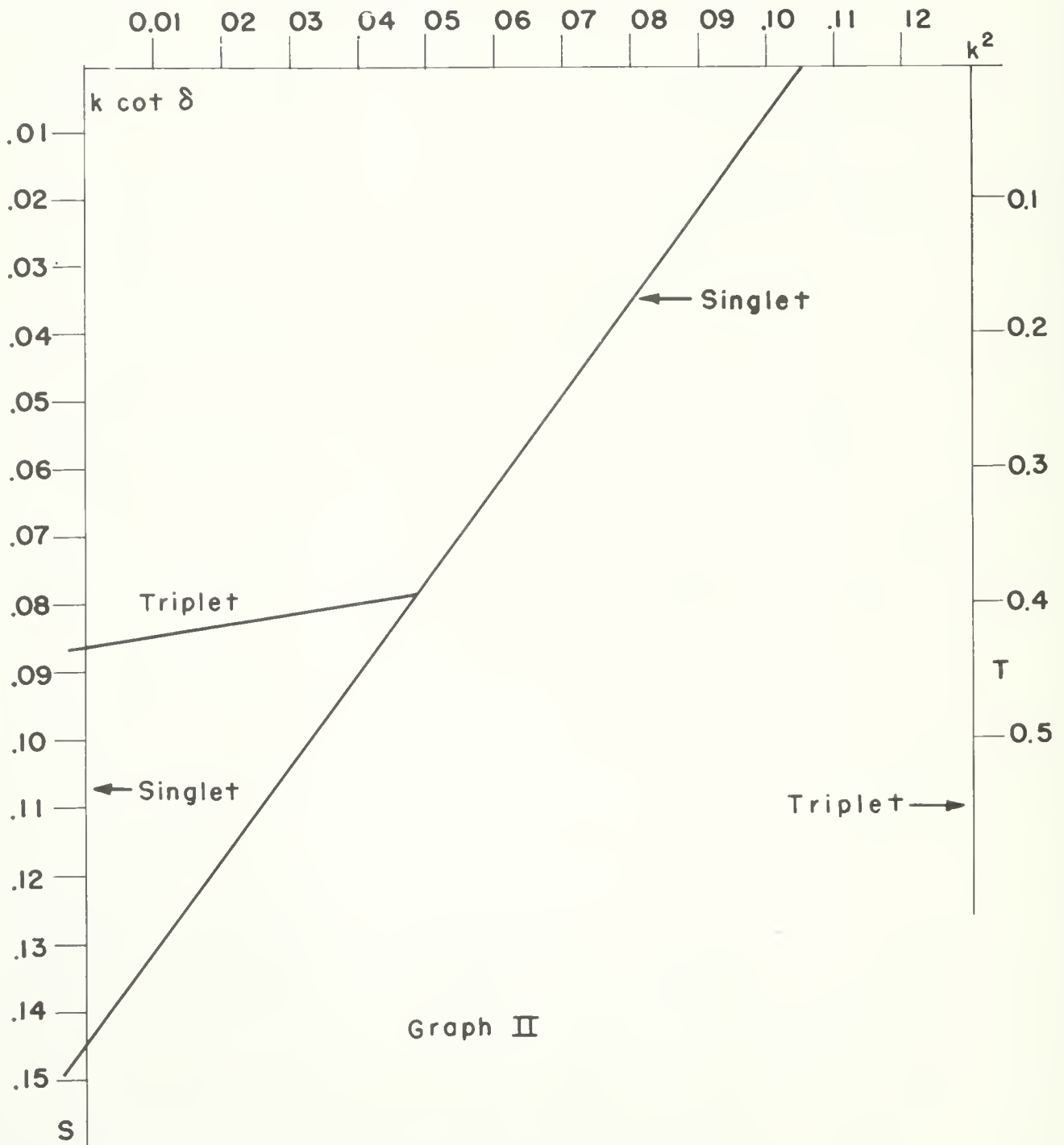
$$\begin{aligned}
& - \frac{4}{(1+\gamma)^2(2+\gamma)^4} + \frac{1}{8(1+2\gamma)^2(1+\gamma)^4} - \frac{2}{(2+\gamma)^4} + \frac{1}{4(1+\gamma)^6} - \frac{2}{(1+2\gamma)^2(2+3\gamma)^4} \\
& + \left(\frac{6\gamma}{(1+\gamma)^4} - \frac{4\gamma^2}{(1+\gamma)^5} \right) \left(1 - \frac{2}{(1+\gamma)^2} + \frac{1}{(1+2\gamma)^2} \right) + \left(\frac{16\gamma^2}{(1+2\gamma)^2} - \frac{8\gamma^2}{(1+\gamma)^2} \right) \left(1 - \frac{1}{(1+\gamma)^5} \right) \\
& - \frac{4}{(2+\gamma)} \left(\frac{1}{(2+\gamma)^3} + \frac{2}{(2+\gamma)^2} + \frac{3}{2+\gamma} + 4 \right) + \frac{1}{(1+\gamma)} \left(\frac{1}{8(1+\gamma)^3} + \frac{1}{2(1+\gamma)^2} + \frac{3}{2(1+\gamma)} + 4 \right) \\
& - \frac{2}{(1+\gamma)^2} \left(\frac{1}{(2+\gamma)} \left(\frac{1}{(2+\gamma)^3} + \frac{2}{(1+\gamma)(2+\gamma)^2} + \frac{3}{(1+\gamma)^2(2+\gamma)} + \frac{4}{(1+\gamma)^3} \right) \right. \\
& \left. - \frac{49}{8(1+\gamma)^4} + \frac{1}{(2+3\gamma)} \left(\frac{1}{(2+3\gamma)^3} + \frac{2}{(1+\gamma)(2+3\gamma)^2} + \frac{3}{(1+\gamma)^2(2+3\gamma)} + \frac{4}{(1+\gamma)^3} \right) \right) \\
& - \frac{6\gamma}{8(1+\gamma)^4} \left(1 - \frac{2}{(1+\gamma)^4} + \frac{1}{(1+2\gamma)^4} \right) - \frac{4}{(1+\gamma)^2(2+\gamma)^2} \left(\frac{3}{(2+\gamma)^2} + \frac{4}{(1+\gamma)(2+\gamma)} \right. \\
& \left. + \frac{3}{(1+\gamma)^2} \right) + \frac{1}{2(1+\gamma)^2(1+2\gamma)^2} \left(\frac{3}{4(1+\gamma)^2} + \frac{2}{(1+\gamma)(1+2\gamma)} + \frac{3}{(1+2\gamma)^2} \right) \\
& - \frac{2}{(2+\gamma)^2} \left(\frac{3}{(2+\gamma)^2} + \frac{4}{(2+\gamma)} + 3 \right) - \frac{2}{(1+2\gamma)^2(2+3\gamma)^2} \left(\frac{3}{(2+3\gamma)^2} + \frac{4}{(1+2\gamma)(2+3\gamma)} \right. \\
& \left. + \frac{3}{(1+2\gamma)^2} \right) + \frac{23}{4(1+\gamma)^6} \Bigg] \cdot
\end{aligned}$$

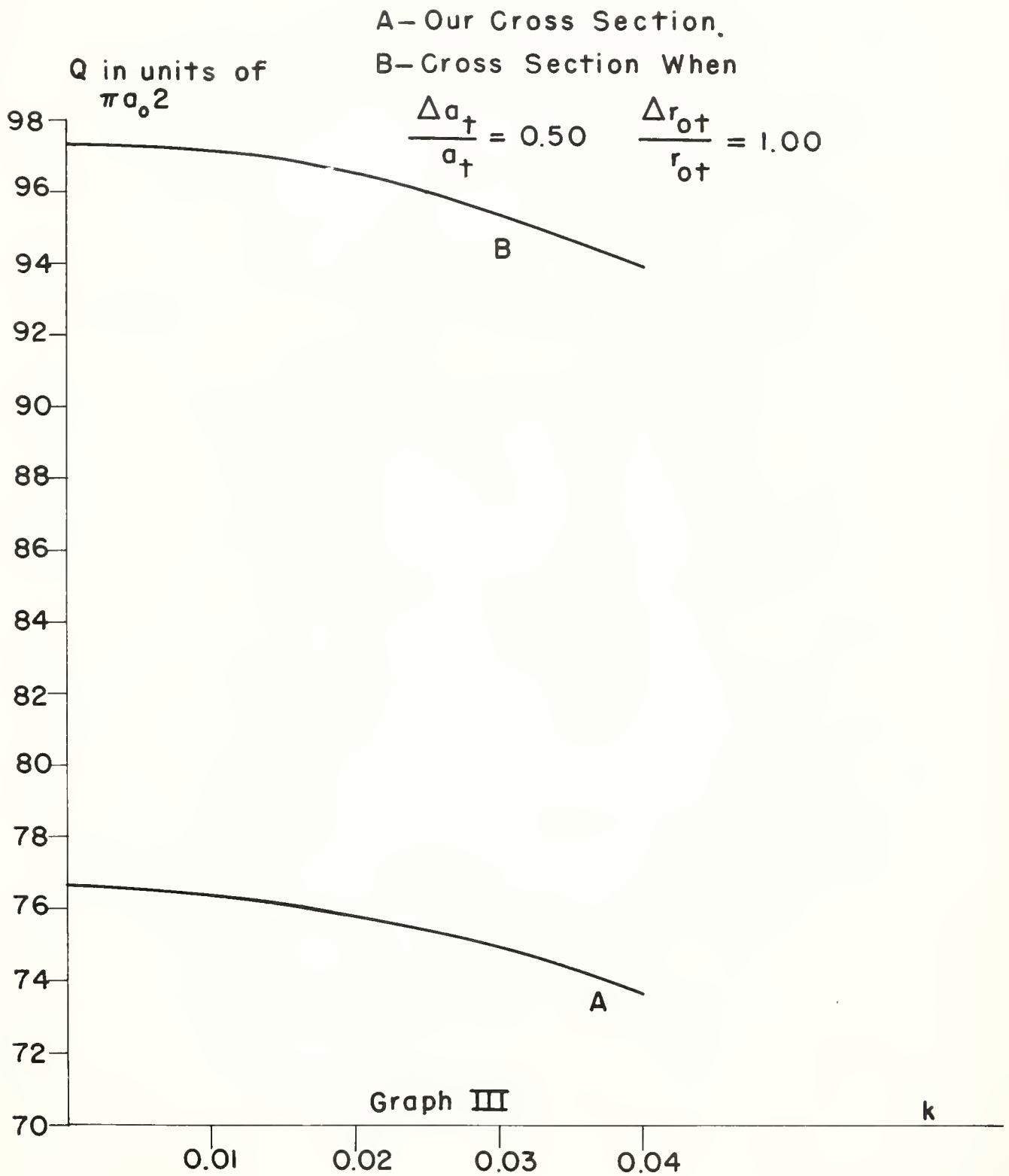
TOTAL CROSS SECTION VS.
WAVE NUMBER



$k \cot \delta$ VS. k^2

FOR CALCULATION BY MASSEY AND MOISEWITSCH

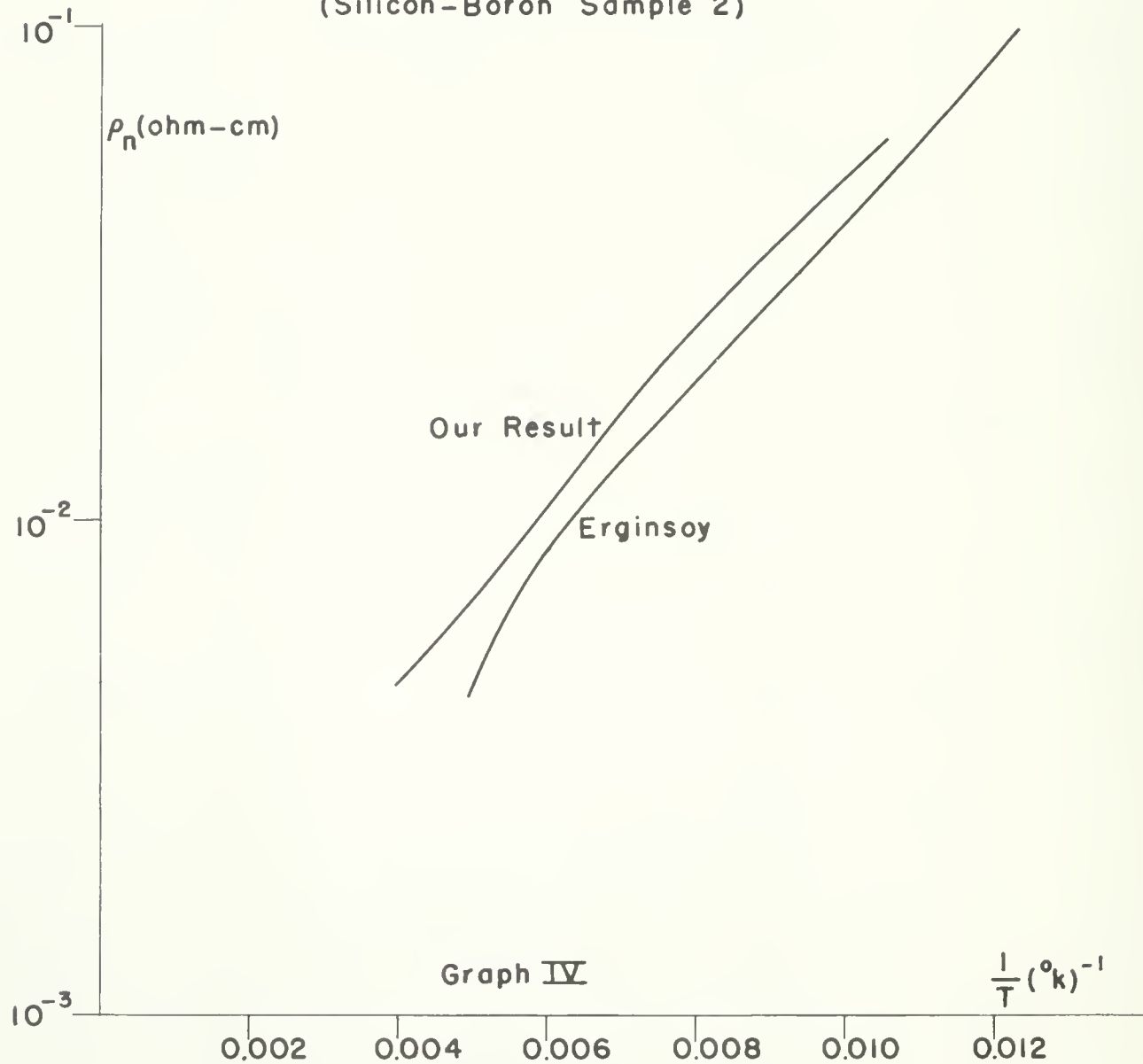




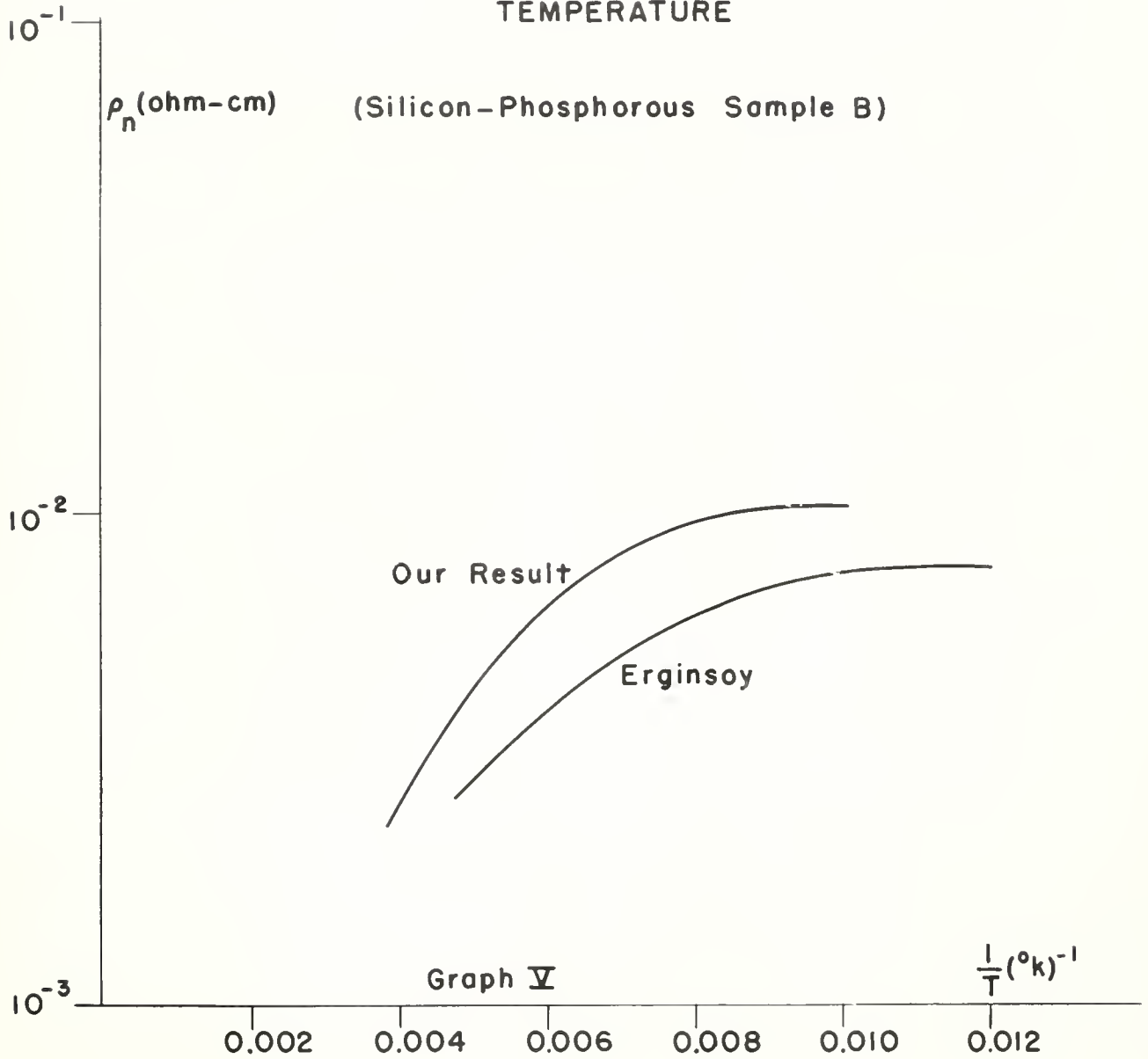
RESISTIVITY VS. INVERSE ABSOLUTE

TEMPERATURE

(Silicon-Boron Sample 2)



RESISTIVITY VS. INVERSE ABSOLUTE
TEMPERATURE



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Greenberg
A Variational Calculation of
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rons by Hydrogen Atoms.

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